GENERAL, ORGANIC, AND BIOCHEMISTRY WITH PROBLEMS, CASE STUDIES, AND ACTIVITIES



LibreTexts™

General, Organic, and Biochemistry with Problems, Case Studies, and Activities

This text is disseminated via the Open Education Resource (OER) LibreTexts Project (https://LibreTexts.org) and like the thousands of other texts available within this powerful platform, it is freely available for reading, printing, and "consuming."

The LibreTexts mission is to bring together students, faculty, and scholars in a collaborative effort to provide an accessible, and comprehensive platform that empowers our community to develop, curate, adapt, and adopt openly licensed resources and technologies; through these efforts we can reduce the financial burden born from traditional educational resource costs, ensuring education is more accessible for students and communities worldwide.

Most, but not all, pages in the library have licenses that may allow individuals to make changes, save, and print this book. Carefully consult the applicable license(s) before pursuing such effects. Instructors can adopt existing LibreTexts texts or Remix them to quickly build course-specific resources to meet the needs of their students. Unlike traditional textbooks, LibreTexts' web based origins allow powerful integration of advanced features and new technologies to support learning.



LibreTexts is the adaptable, user-friendly non-profit open education resource platform that educators trust for creating, customizing, and sharing accessible, interactive textbooks, adaptive homework, and ancillary materials. We collaborate with individuals and organizations to champion open education initiatives, support institutional publishing programs, drive curriculum development projects, and more.

The LibreTexts libraries are Powered by NICE CXone Expert and was supported by the Department of Education Open Textbook Pilot Project, the California Education Learning Lab, the UC Davis Office of the Provost, the UC Davis Library, the California State University Affordable Learning Solutions Program, and Merlot. This material is based upon work supported by the National Science Foundation under Grant No. 1246120, 1525057, and 1413739.

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation nor the US Department of Education.

Have questions or comments? For information about adoptions or adaptions contact info@LibreTexts.org or visit our main website at https://LibreTexts.org.

This text was compiled on 01/12/2026

Preface

The Creation of this Open Educational Resource (OER)

This textbook and ancillary materials were created as part of the Illinois Support for the Creation of Open Educational Resources (SCOERs) project, facilitated by the Consortium of Academic and Research Libraries in Illinois (CARLI) and funded by a $2 million Open Textbooks Pilot Program grant from the Department of Education and the Fund for the Improvement of Post-Secondary Education

The contents of this publication were developed under a grant from the Fund for the Improvement of Postsecondary Education, (FIPSE), U.S. Department of Education. However, those contents do not necessarily represent the policy of the Department of Education, and you should not assume endorsement by the Federal Government.

Illinois SCOERs is a true statewide enterprise fundamentally changing the open educational resources landscape in Illinois by providing a new holistic support model that promotes student success through OER awareness, implementation, growth, and adoption. This project features a collaboration between educational systems in Illinois, the library community, and workforce representatives. Developed OER course materials will be released under a license that permits their free use, reuse, modification, and sharing with others., the library community, and workforce representatives. Developed OER course materials will be released under a license that permits their free use, reuse, modification, and sharing with others.

About this Book

This book and its ancillary materials were made possible through an Illinois SCOERs Subgrant awarded to Roosevelt University, DePaul University and Harper College. The materials created for the General, Organic, and Biochemistry (GOB) Nursing Classes at the institutions, a high enrollment course for undergraduate/graduate students.

Editors

- Richard Niedziela, Associate Professor of Chemistry, DePaul University
- Josh Telser, Associate Professor of Chemistry, Roosevelt University

Developing Authors

Developing authors remix existing OER and create content from evidence-based sources that are aligned with the Illinois Board of Higher Education.

- Tim French, Associate Professor of Chemistry, DePaul University, Author
- Kyle Grice, Associate Professor of Chemistry, DePaul University, Author
- Luisel Lemkau, Assistant Professor of Chemistry, Harper College, Author
- Bob Seiser, Chair of Biology, Physics, and Health Sciences, Roosevelt University, Author
- Carrie Southern, Associate Professor of Chemistry, DePaul University, Author
- Joe Wachter, Professor of Chemistry, Harper College, Author
- Roxanne Spurlank, Assistant Director of Advanced Practice Nursing, DePaul University, Industry Sector Representative and Author

Contributors

Contributors to the development of this OER textbook/ancillary materials include educators, librarians, and staff from Roosevelt University, DePaul University, and Harper College:

- Barbara Anderson, Instructional Librarian, Roosevelt University, Principal Investigator
- Chris Dobson, Instructional Media Developer, DePaul University, Instructional Designer
- April Hummons, Information Technology Librarian, DePaul University, 3D Printing Coordinator
- Thom Jencks, Performing Arts Librarian, Roosevelt University, Copyright Coordinator
- Wills Waites, Instruction and Access Service Librarian, Roosevelt University, Copyright Coordinator

- Ashley McMullin, Associate University Librarian for Teaching, Research, and Engagement, DePaul University, Accessibility Coordinator
- Susan Shultz, Business and Social Science Librarian, DePaul University, Accessibility Coordinator

Illinois SCOERs Project Staff

The Illinois SCOERs Project Staff helped coordinate the management of the Open Textbook Pilot grant that made this OER possible. Topical experts shared their knowledge on open educational resources, incorporating technologies including 3D printing, accessibility, author rights, instructional design, publishing, and participated with the review and proofreading processes.

- Anne Craig, Principal Investigator, CARLI Senior Director
- Michele Leigh, Project Director, CARLI Senior Coordinator Open Illinois
- Margaret Chambers, CARLI Director and Advisor, Membership and Communications
- Michelle Haake, CARLI Senior Coordinator Membership and Communications
- Diane Day, CARLI Fiscal Officer
- Elizabeth Clarage, CARLI Director, Collections Services and OER Committee Liaison
- Nicole Swanson, CARLI Senior Coordinator, Library Services and Outreach and OER Committee Liaison
- Sara Benson, Copyright Training Coordinator, Assistant Professor, Copyright Librarian, University of Illinois Urbana-Champaign
- Emily Boles, Instructional Design Coordinator and Trainer, eLearning Specialist, University of Illinois Springfield
- Elisandro (Alex) Cabada, 3D Printing Coordinator Trainer, Assistant Professor and Medical & Bioengineering Librarian, University of Illinois Urbana-Champaign
- Ann Fredricksen, Disability Specialist, Coordinator of Accessible Media Services, University of Illinois Urbana-Champaign, Disability Resources and Educational Services (DRES)
- Kathleen Ricker, Proofreader, ProofreadingPal.com Editing Services

Advisory Committee

The Illinois SCOERs Advisory Committee provided input on the subgrant applications, and the materials produced and contains industry members, librarians, graduate students, and representatives from our project partners:

- Illinois Community College Board
- Illinois Board of Higher Education
- Illinois Department of Commerce & Economic Opportunity
- Illinois Heartland Library System
- Reaching Across Illinois Library System
- Illinois State Library
- Illinois Library Association
- Health Sciences Librarians of Illinois
- University of Illinois Urbana-Champaign's Division of Disability Resources and Educational Services
- Laurie Brown, Executive Director, Hickory Point Christian Village (assisted living) and Illinois Workforce Investment Board Local 1949 Chair
- Lisa Jones, DCEO, Manager, Office of Employment & Training (state workforce agency)
- Suzanne Kinsey, Executive Director, Fox Valley Community Services, (in-home service agency) in DeKalb, LaSalle, Kendall, and Kane Counties
- Danna Williamson, Nursing Education Specialist, Carle Foundation Hospital Clinical Education

Peer Review

The Peer Reviewer process was completed by the following reviewers:

Request to Those Using This Resource: Usage Survey

We would love to hear if you have integrated some, or all of this resource into your course. Please submit usage information every semester for grant reporting purposes using this short survey. Your personal information will be kept private and only the usage

data will be shared with the Department of Education.

Customization/Terms of Use

This textbook is licensed under a Creative Commons Attribution 4.0 International (CC-BY) license unless otherwise indicated, which means that you are free to:

- SHARE – copy and redistribute the material in any medium or format
- ADAPT – remix, transform, and build upon the material for any purpose

Licensing Terms

The licensor cannot revoke these freedoms as long as you follow the license terms.

- Attribution: You must give appropriate credit, provide a link to the license, and indicate if any changes were made. You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use.
- No Additional Restrictions: You may not apply legal terms or technological measures that legally restrict others from doing anything the license permits.
- Notice: You do not have to comply with the license for elements of the material in the public domain or where your use is permitted by an applicable United States copyright exception or limitation.
- No Warranties are Given: The license may not give you all of the permissions necessary for your intended use. For example, other rights such as publicity, privacy, or moral rights may limit how you use the material.

Attribution

Some of the content for this textbook was adapted from the following open educational resources. For specific reference information about what was used and/or changed in this adaptation, please refer to the footnotes at the bottom of each page of the book.

Suggested Attribution Statement for this Book

Content that is not taken from the OER on the References should include the following attribution statement:

French, T. A., Grice K. A., Lemkau, L. R., Seiser, R. M., Southern, C. A., Spurlark, R. S, & Wachter, J. B. (2023). Illinois SCOERs. General, Organic, and Biochemistry with Problems, Case Studies, and Activities by Consortium of Academic and Research Libraries in Illinois licensed under CC BY 4.0.

References

This Preface chapter is a derivative of Ernstmeyer, K., & Christman, E. (Eds.). (2022). Nursing Mental Health and Community Concepts by Chippewa Valley Technical College is licensed under CC BY 4.0

Avril, B. & Eldredge, P. (2011). General Chemistry: Principles, Patterns, and Applications. Open Textbook Library. Retrieved September 15, 2023.

Ball, D., Hill, J., & Scott, R. (2022, July 13). Basics of General, Organic, and Biological Chemistry. LibreTexts. Retrieved September 15, 2023.

Brown, T., LeMay, H., Bursten, B., Murphy, C., & Woodward, P. (2021, May 19). Map Chemistry: The Central Science. LibreTexts. Retrieved September 15, 2023.

Clark, M., Douglas, M, & Choi, J. (2018, March 28). Biology 2e. OpenStax. Retrieved September 15, 2023.

Doyle, G., McCutcheon, J. (n.d.). Clinical Procedures for Safer Patient Care. LibreTexts. Retrieved September 15, 2023.

Ernstmeyer & Christman. (Eds.). (n.d.). Nursing Fundamentals (OpenRN). LibreTexts. Retrieved September 15, 2023.

Flowers, P., Theopold, K., Langley, R., & Robinson, W. (2023, June 28). Chemistry 2e. OpenStax. Retrieved September 15, 2023.

General Biology (Boundless). (n.d.). LibreTexts. Retrieved September 15, 2023.

Harper College Chemistry Department. (n.d.). Chemistry for the Health Sciences. Pressbooks. Retrieved September 15, 2023.

Lower, S. (2022, February 20). Chem1e. LibreTexts. Retrieved September 15, 2023.

Parker, N., Schneegurt, M., Tu, A., Lister, P., & Forster, B. (2016, November 1). Microbiology. OpenStax. Retrieved September 15, 2023.

Reusch, W. (1999). Virtual Textbook of Organic Chemistry. Retrieved September 15, 2023.

Soderberg, T. (2021, September 12). Organic Chemistry with a Biological Emphasis. LibreTexts. Retrieved September 15, 2023.

TABLE OF CONTENTS

Preface

Licensing

1: Scientific Method, Matter, and Measurements

- 1.1: The Scientific Method
- 1.2: Units
- 1.3: Matter
- 1.4: Physical and Chemical Properties
- 1.5: Case Study- Using the Scientific Method to Diagnose an Autoimmune Disorder
- 1.E: Exercises

2: Atoms and Elements

- 2.1: Atomic Theory
- 2.2: Atomic Structure
  - 2.2.1: Nuclei of Atoms
- 2.3: Atomic Masses
- 2.4: Electronic Structure in Atoms
- 2.5: The Periodic Table
- 2.6: Health Connections- Essential Elements for Life
- 2.7: Case Study- Electrons and Electronic Structure in Medical Applications
- 2.8: 3D Printing Activity - Periodic Trends
- 2.E: Exercises

3: Ionic and Covalent Compounds

- 3.1: Molecular and Ionic Compounds
- 3.2: Ionic Bonding
- 3.3: Covalent Bonding
- 3.4: Chemical Nomenclature
- 3.5: Case Study- Ionic and Covalent Compounds in Biochemistry
- 3.E: Exercises

4: Chemical Bonding

- 4.1: Lewis Symbols and Structures
- 4.2: Formal Charges and Resonance
- 4.3: Molecular Structure and Polarity
- 4.4: Valence Bond Theory
- 4.5: Hybrid Atomic Orbitals
- 4.6: Multiple Bonds
- 4.7: Case Study- Chemical Bonding - Deciphering Drug Interactions through Lewis Structures
- 4.8: 3D Printing Activity- VSEPR and Ionic/Metallic Solids Structures
- 4.E: Exercises

5: Unit Conversions

- 5.1: Density and Temperature
  - 5.1.1: Mathematical Treatment of Measurement Results
- 5.2: Measurement Uncertainty, Accuracy, and Precision
- 5.3: Unit Conversions
- 5.4: Health Connections- Dosage Calculations
- 5.5: Case Study- Precision in Pediatric Care – The Imperative of Unit Conversion
- 5.E: Exercises

6: Moles

- 6.1: The Mole
- 6.2: Formula Mass
- 6.3: Converting between Grams and Moles
- 6.4: Case Study- The Mole Concept in Clinical Laboratory Analysis
- 6.E: Exercises

7: Chemical Equations and Reactions

- 7.1: Balancing Chemical Equations
- 7.2: Energy Basics
- 7.3: Chemical Equilibrium
- 7.4: Catalysis
- 7.5: Case Study- Balancing Acts in Pharmacological Synthesis
- 7.E: Exercises

8: Gases, Liquids, and Solids

- 8.1: The Kinetic-Molecular Theory
- 8.2: Gas Pressure
- 8.3: The Gas Laws
- 8.4: Intermolecular Forces
- 8.5: Types of Solutions
- 8.6: Electrolytes
- 8.7: Concentration
  - 8.7.1: Other Units for Solution Concentrations
- 8.8: Osmosis, Diffusion and Dialysis
- 8.9: Health Connections- Oxygen in the Body
- 8.10: Case Study- The Vital Breath – Kinetic Molecular Theory in Respiratory Care
- 8.E: Exercises

9: Acids and Bases

- 9.1: What are Acids and Bases?
- 9.2: pH and pOH
- 9.3: Acid-Base Balance
- 9.4: Case Study- Navigating the Delicate pH Spectrum in Intensive Care
- 9.E: Exercises

10: Introduction to Organic Chemistry

- 10.1: Drawing organic structures
- 10.2: Alkanes and isomers
- 10.3: Functional groups
- 10.4: Case Study- The Molecular Tapestry of Healing
- 10.5: 3D Printing Activity- Cyclohexane
- 10.E: Exercises

11: Organic Chemistry Reactions

- 11.1: Organic Reactions
- 11.2: Alcohols and Ethers
- 11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters
- 11.4: Amines and Amides
- 11.E: Exercises

12: Carbohydrates

- 12.1: Carbohydrates
- 12.2: Fischer and Haworth projections
- 12.3: Case Study- Tailoring Nutrition – Carbohydrates in Diabetes Care
- 12.E: Exercises

13: Lipids

- 13.1: Lipids
- 13.2: Case Study- Lipids and Heart Health - Interpreting Lipid Profiles
- 13.E: Exercises

14: Proteins

- 14.1: Properties of Proteins
- 14.2: Amino Acids
- 14.3: Primary Structure- Peptides
- 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
- 14.5: Case Study- Synergy in Science and Care - Protein Structures Illuminating Metabolic Disorder Management
- 14.6: 3D Printing Activity- Protein-Ligand Binding
- 14.E: Exercises

15: Molecular Genetics

- 15.1: DNA Structure
- 15.2: Case Study- Decoding Disease - The Role of DNA Structure in Genetic Disorders
- 15.E: Exercises

16: Answers to Odd Problems

- 16.1: Ch. 1 Odd Answers
- 16.2: Ch. 2 Odd Answers
- 16.3: Ch. 3 Odd Answers
- 16.4: Ch. 4 Odd Answers
- 16.5: Ch. 5 Odd Answers
- 16.6: Ch. 6 Odd Answers

- 16.7: Ch. 7 Odd Answers
- 16.8: Ch. 8 Odd Answers
- 16.9: Ch. 9 Odd Answers
- 16.10: Ch. 10 Odd Answers
- 16.11: Ch. 11 Odd Answers
- 16.12: Ch. 12 Odd Answers
- 16.13: Ch. 13 Odd Answers
- 16.14: Ch. 14 Odd Answers
- 16.15: Ch. 15 Odd Answers

Index

Glossary

Detailed Licensing

Licensing

*A detailed breakdown of this resource's licensing can be found in **Back Matter/Detailed Licensing**.*

CHAPTER OVERVIEW

1: Scientific Method, Matter, and Measurements

1.1: The Scientific Method

1.2: Units

1.3: Matter

1.4: Physical and Chemical Properties

1.5: Case Study- Using the Scientific Method to Diagnose an Autoimmune Disorder

1.E: Exercises

1: Scientific Method, Matter, and Measurements is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

1.1: The Scientific Method

Learning Objectives

By the end of this section, you will be able to

- Outline the historical development of chemistry
- Provide examples of the importance of chemistry in everyday life
- Describe the scientific method
- Differentiate among hypotheses, theories, and laws
- Provide examples illustrating macroscopic, microscopic, and symbolic domains

Throughout human history, people have tried to convert matter into more useful forms. Our Stone Age ancestors chipped pieces of flint into useful tools and carved wood into statues and toys. These endeavors involved changing the shape of a substance without changing the substance itself. But as our knowledge increased, humans began to change the composition of the substances as well—clay was converted into pottery, hides were cured to make garments, copper ores were transformed into copper tools and weapons, and grain was made into bread.

Humans began to practice chemistry when they learned to control fire and use it to cook, make pottery, and smelt metals. Subsequently, they began to separate and use specific components of matter. A variety of drugs, such as aloe, myrrh, and opium, were isolated from plants. Dyes, such as indigo and Tyrian purple, were extracted from plant and animal matter. Metals were combined to form alloys—for example, copper and tin were mixed together to make bronze—and more elaborate smelting techniques produced iron. Alkalis were extracted from ashes, and soaps were prepared by combining these alkalis with fats. Alcohol was produced by fermentation and purified by distillation.

Attempts to understand the behavior of matter extend back for more than 2500 years. As early as the sixth century BC, Greek philosophers discussed a system in which water was the basis of all things. You may have heard of the Greek postulate that matter consists of four elements: earth, air, fire, and water. Subsequently, an amalgamation of chemical technologies and philosophical speculations was spread from Egypt, China, and the eastern Mediterranean by alchemists, who endeavored to transform “base metals” such as lead into “noble metals” like gold, and to create elixirs to cure disease and extend life (Figure **1.1.1**).

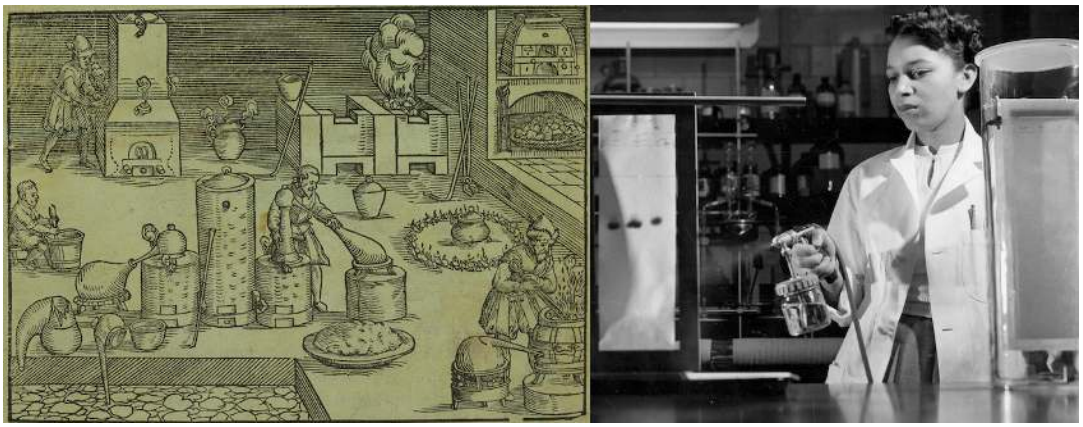


Figure **1.1.1**: (a) This portrayal shows an alchemist’s workshop circa 1580. Although alchemy made some useful contributions to how to manipulate matter, it was not scientific by modern standards. (b) While the equipment used by Alma Levant Hayden in this 1952 picture might not seem as sleek as you might find in a lab today, her approach was highly methodical and carefully recorded. A department head at the FDA, Hayden is most famous for exposing an aggressively marketed anti-cancer drug as nothing more than an unhelpful solution of common substances. (credit a: Chemical Heritage Foundation; b: NIH History Office)

From alchemy came the historical progressions that led to modern chemistry: the isolation of drugs from natural sources, such as plants and animals. But while many of the substances extracted or processed from those natural sources were critical in the treatment of diseases, many were scarce. For example, progesterone, which is critical to women's health, became available as a medicine in 1935, but its animal sources produced extremely small quantities, limiting its availability and increasing its expense. Likewise, in the 1940s, cortisone came into use to treat arthritis and other disorders and injuries, but it took a 36-step process to

synthesize. Chemist Percy Lavon Julian turned to a more plentiful source: soybeans. Previously, Julian had developed a lab to isolate soy protein, which was used in firefighting, among other applications. He focused on using the soy sterols—substances mostly used in plant membranes—and was able to quickly produce progesterone and later testosterone and other hormones. He later developed a process to do the same for cortisone and laid the groundwork for modern drug design. Since soybeans and similar plant sources were extremely plentiful, the drugs soon became widely available, saving many lives.

1.1.1: Chemistry: The Central Science

Chemistry is sometimes referred to as “the central science” due to its interconnectedness with a vast array of other STEM disciplines (STEM stands for areas of study in the science, technology, engineering, and math fields). Chemistry and the language of chemists play vital roles in biology, medicine, materials science, forensics, environmental science, and many other fields (Figure **1.1.2**). The basic principles of physics are essential for understanding many aspects of chemistry, and there is extensive overlap between many subdisciplines within the two fields, such as chemical physics and nuclear chemistry. Mathematics, computer science, and information theory provide important tools that help us calculate, interpret, describe, and generally make sense of the chemical world. Biology and chemistry converge in biochemistry, which is crucial to understanding the many complex factors and processes that keep living organisms (such as us) alive. Chemical engineering, materials science, and nanotechnology combine chemical principles and empirical findings to produce useful substances, ranging from gasoline to fabrics to electronics. Agriculture, food science, veterinary science, brewing, and wine-making help provide sustenance in the form of food and drink to the world’s population. Medicine, pharmacology, biotechnology, and botany identify and produce substances that help keep us healthy. Environmental science, geology, oceanography, and atmospheric science incorporate many chemical ideas to help us better understand and protect our physical world. Chemical ideas are used to help understand the universe in astronomy and cosmology.

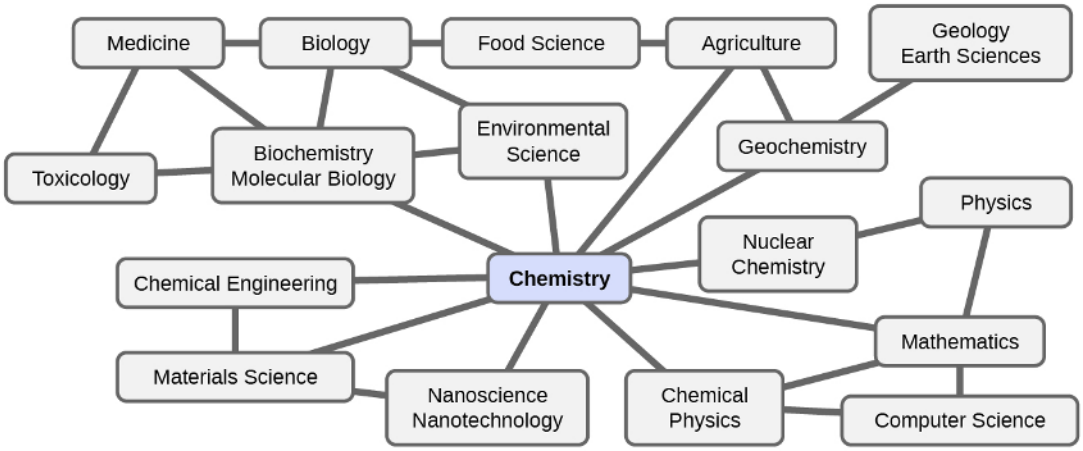


Figure **1.1.2**: Knowledge of chemistry is central to understanding a wide range of scientific disciplines. This diagram shows just some of the interrelationships between chemistry and other fields.

What are some changes in matter that are essential to daily life? Digesting and assimilating food, synthesizing polymers that are used to make clothing, containers, cookware, and credit cards, and refining crude oil into gasoline and other products are just a few examples. As you proceed through this course, you will discover many different examples of changes in the composition and structure of matter, how to classify these changes and how they occurred, their causes, the changes in energy that accompany them, and the principles and laws involved. As you learn about these things, you will be learning chemistry, the study of the composition, properties, and interactions of matter. The practice of chemistry is not limited to chemistry books or laboratories: It happens whenever someone is involved in changes in matter or in conditions that may lead to such changes.

1.1.2: The Scientific Method

Chemistry is a science based on observation and experimentation. Doing chemistry involves attempting to answer questions and explain observations in terms of the laws and theories of chemistry, using procedures that are accepted by the scientific community. There is no single route to answering a question or explaining an observation, but there is an aspect common to every approach: Each uses knowledge based on experiments that can be reproduced to verify the results. Some routes involve a hypothesis, a

tentative explanation of observations that acts as a guide for gathering and checking information. A hypothesis is tested by experimentation, calculation, and/or comparison with the experiments of others and then refined as needed.

Some hypotheses are attempts to explain the behavior that is summarized in laws. The laws of science summarize a vast number of experimental observations and describe or predict some facet of the natural world. If such a hypothesis turns out to be capable of explaining a large body of experimental data, it can reach the status of a theory. Scientific theories are well-substantiated, comprehensive, testable explanations of particular aspects of nature. Theories are accepted because they provide satisfactory explanations, but they can be modified if new data become available. The path of discovery that leads from question and observation to law or hypothesis to theory, combined with experimental verification of the hypothesis and any necessary modification of the theory, is called the scientific method (Figure **1.1.3**).

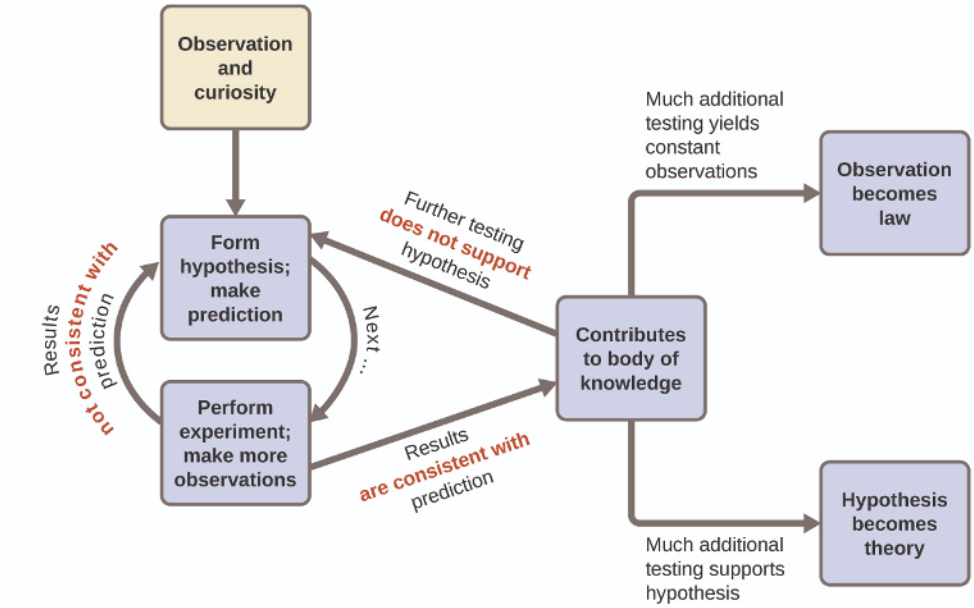


Figure **1.1.3**: The scientific method follows a process similar to the one shown in this diagram. All the key components are shown, in roughly the right order. Scientific progress is seldom neat and clean: It requires open inquiry and the reworking of questions and ideas in response to findings.

1.1.3: The Domains of Chemistry

Chemists study and describe the behavior of matter and energy in three different domains: macroscopic, microscopic, and symbolic. These domains provide different ways of considering and describing chemical behavior.

Macro is a Greek word that means “large.” The macroscopic domain is familiar to us: It is the realm of everyday things that are large enough to be sensed directly by human sight or touch. In daily life, this includes the food you eat and the breeze you feel on your face. The macroscopic domain includes everyday and laboratory chemistry, where we observe and measure physical and chemical properties such as density, solubility, and flammability.

Micro comes from Greek and means “small.” The microscopic domain of chemistry is often visited in the imagination. Some aspects of the microscopic domain are visible through standard optical microscopes, for example, many biological cells. More sophisticated instruments are capable of imaging even smaller entities such as molecules and atoms (see Figure **1.1.4**: (**b**)).

However, most of the subjects in the microscopic domain of chemistry are too small to be seen even with the most advanced microscopes and may only be pictured in the mind. Other components of the microscopic domain include ions and electrons, protons and neutrons, and chemical bonds, each of which is far too small to see.

The symbolic domain contains the specialized language used to represent components of the macroscopic and microscopic domains. Chemical symbols (such as those used in the periodic table), chemical formulas, and chemical equations are part of the symbolic domain, as are graphs, drawings, and calculations. These symbols play an important role in chemistry because they help interpret the behavior of the macroscopic domain in terms of the components of the microscopic domain. One of the challenges for students learning chemistry is recognizing that the same symbols can represent different things in the macroscopic and microscopic

domains, and one of the features that makes chemistry fascinating is the use of a domain that must be imagined to explain behavior in a domain that can be observed.

A helpful way to understand the three domains is via the essential and ubiquitous substance of water. That water is a liquid at moderate temperatures, will freeze to form a solid at lower temperatures, and boil to form a gas at higher temperatures (Figure **1.1.4**) are macroscopic observations. But some properties of water fall into the microscopic domain—what cannot be observed with the naked eye. The description of water as comprising two hydrogen atoms and one oxygen atom, and the explanation of freezing and boiling in terms of attractions between these molecules, is within the microscopic arena. The formula H_2O, which can describe water at either the macroscopic or microscopic levels, is an example of the symbolic domain. The abbreviations (*g*) for gas, (*s*) for solid, and (*l*) for liquid are also symbolic.

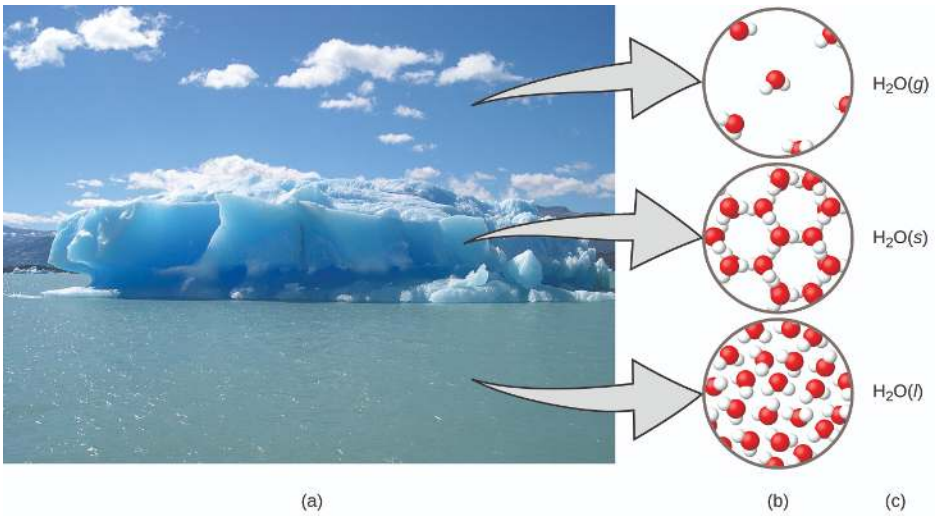


Figure **1.1.4**: (a) Moisture in the air, icebergs, and the ocean represent water in the macroscopic domain. (b) At the molecular level (microscopic domain), gas molecules are far apart and disorganized, solid water molecules are close together and organized, and liquid molecules are close together and disorganized. (c) The formula H_2O symbolizes water, and (*g*), (*s*), and (*l*) symbolize its phases. Note that clouds are actually comprised of either very small liquid water droplets or solid water crystals; gaseous water in our atmosphere is not visible to the naked eye, although it may be sensed as humidity. (credit a: modification of work by "Gorkaazk"/Wikimedia Commons)

This page titled 1.1: The Scientific Method is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

1.2: Units

Learning Objectives

By the end of this section, you will be able to:

- Explain the process of measurement
- Identify the three basic parts of a quantity
- Describe the properties and units of length, mass, volume, density, temperature, and time
- Perform basic unit calculations and conversions in the metric and other unit systems

Measurements provide much of the information that informs the hypotheses, theories, and laws describing the behavior of matter and energy in both the macroscopic and microscopic domains of chemistry. Every measurement provides three kinds of information: the size or magnitude of the measurement (a number); a standard of comparison for the measurement (a unit); and an indication of the uncertainty of the measurement. While the number and unit are explicitly represented when a quantity is written, the uncertainty is an aspect of the measurement result that is more implicitly represented and will be discussed later.

The number in the measurement can be represented in different ways, including decimal form and scientific notation. (Scientific notation is also known as exponential notation; a review of this topic can be found in Appendix B.) For example, the maximum takeoff weight of a Boeing 777-200ER airliner is 298,000 kilograms, which can also be written as $2.98\ 10^5$ kg. The mass of the average mosquito is about 0.0000025 kilograms, which can be written as $2.5\ 10^{-6}$ kg.

Units, such as liters, pounds, and centimeters, are standards of comparison for measurements. A 2-liter bottle of a soft drink contains a volume of beverage that is twice that of the accepted volume of 1 liter. The meat used to prepare a 0.25-pound hamburger weighs one-fourth as much as the accepted weight of 1 pound. Without units, a number can be meaningless, confusing, or possibly life threatening. Suppose a doctor prescribes phenobarbital to control a patient's seizures and states a dosage of "100" without specifying units. Not only will this be confusing to the medical professional giving the dose, but the consequences can be dire: 100 mg given three times per day can be effective as an anticonvulsant, but a single dose of 100 g is more than 10 times the lethal amount.

The measurement units for seven fundamental properties ("base units") are listed in Table **1.2.1**. The standards for these units are fixed by international agreement, and they are called the **International System of Units** or SI Units (from the French, *Le Système International d'Unités*). SI units have been used by the United States National Institute of Standards and Technology (NIST) since 1964. Units for other properties may be derived from these seven base units.

Table **1.2.1**: Base Units of the SI System

Property Measured	Name of Unit	Symbol of Unit
length	meter	m
mass	kilogram	kg
time	second	s
temperature	kelvin	K
electric current	ampere	A
amount of substance	mole	mol
luminous intensity	candela	cd

Everyday measurement units are often defined as fractions or multiples of other units. Milk is commonly packaged in containers of 1 gallon (4 quarts), 1 quart (0.25 gallon), and one pint (0.5 quart). This same approach is used with SI units, but these fractions or multiples are always powers of 10. Fractional or multiple SI units are named using a prefix and the name of the base unit. For

example, a length of 1000 meters is also called a kilometer because the prefix *kilo* means “one thousand,” which in scientific notation is 10^3 (1 kilometer = 1000 m = 10^3 m). The prefixes used and the powers to which 10 are raised are listed in Table **1.2.2**.

Table **1.2.2**: Common Unit Prefixes

Prefix	Symbol	Factor	Example
femto	f	10^{-15}	1 femtosecond (fs) = 1 x 10^{-15} s (0.000000000000001 s)
pico	p	10^{-12}	1 picometer (pm) = 1 x 10^{-12} m (0.000000000001 m)
nano	n	10^{-9}	4 nanograms (ng) = 4 x 10^{-9} g (0.000000004 g)
micro	μ	10^{-6}	1 microliter (μL) = 1 x 10^{-6} L (0.000001 L)
milli	m	10^{-3}	2 millimoles (mmol) = 2 x 10^{-3} mol (0.002 mol)
centi	c	10^{-2}	7 centimeters (cm) = 7 x 10^{-2} m (0.07 m)
deci	d	10^{-1}	1 deciliter (dL) = 1 x 10^{-1} L (0.1 L)
kilo	k	10^{3}	1 kilometer (km) = 1 x 10^{3} m (1000 m)
mega	M	10^{6}	3 megahertz (MHz) = 3 x 10^{6} Hz (3,000,000 Hz)
g	G	10^{9}	8 gigayears (Gyr) = 8 x 10^{9} yr

Prefix	Symbol	Factor	Example
giga			(8,000,000,000 yr)
tera	T	10^{12}	5 terawatts (TW) = 5 x 10^{12} W (5,000,000,000,000 W)

Link to Learning

Need a refresher or more practice with scientific notation? Visit this site to go over the basics of scientific notation.

1.2.1: SI Base Units

The initial units of the metric system, which eventually evolved into the SI system, were established in France during the French Revolution. The original standards for the meter and the kilogram were adopted there in 1799 and eventually by other countries. This section introduces four of the SI base units commonly used in chemistry. Other SI units will be introduced in subsequent chapters.

1.2.1.1: Length

The standard unit of **length** in both the SI and original metric systems is the **meter** (m). A meter was originally specified as 1/10,000,000 of the distance from the North Pole to the equator. It is now defined as the distance light in a vacuum travels in 1/299,792,458 of a second. A meter is about 3 inches longer than a yard (Figure **1.2.1**); one meter is about 39.37 inches or 1.094 yards. Longer distances are often reported in kilometers (1 km = 1000 m = 10^3 m), whereas shorter distances can be reported in centimeters (1 cm = 0.01 m = 10^{-2} m) or millimeters (1 mm = 0.001 m = 10^{-3} m).

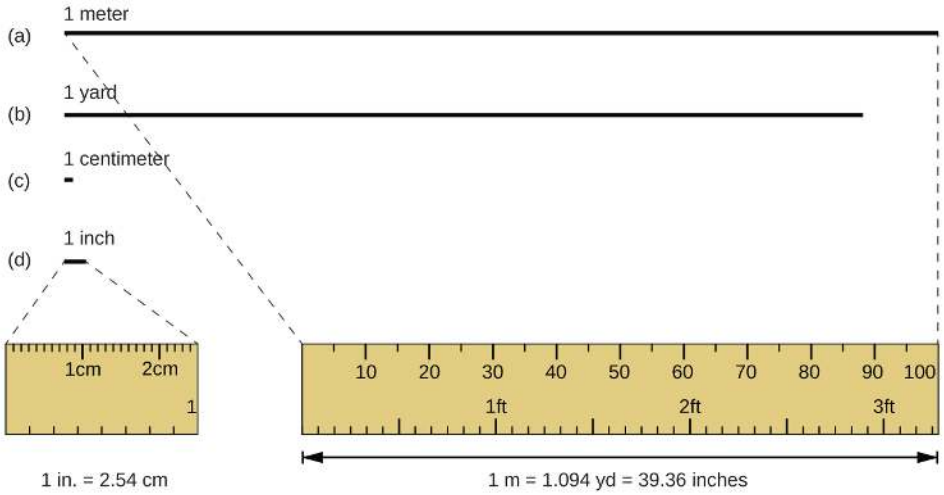


Figure **1.2.1**: The relative lengths of 1 m, 1 yd, 1 cm, and 1 in. are shown (not actual size), as well as comparisons of 2.54 cm and 1 in., and of 1 m and 1.094 yd.

1.2.1.2: Mass

The standard unit of mass in the SI system is the **kilogram** (kg). The kilogram was previously defined by the International Union of Pure and Applied Chemistry (IUPAC) as the mass of a specific reference object. This object was originally one liter of pure water, and more recently it was a metal cylinder made from a platinum-iridium alloy with a height and diameter of 39 mm (Figure **1.2.2**). In May 2019, this definition was changed to one that is based instead on precisely measured values of several fundamental physical constants.[1]. One kilogram is about 2.2 pounds. The gram (g) is exactly equal to 1/1000 of the mass of the kilogram (10^{-3} kg).



Figure **1.2.2**: This replica prototype kilogram as previously defined is housed at the National Institute of Standards and Technology (NIST) in Maryland. (credit: National Institutes of Standards and Technology)

1.2.1.3: Temperature

Temperature is an intensive property. The SI unit of temperature is the kelvin (K). The IUPAC convention is to use **kelvin** (all lowercase) for the word, K (uppercase) for the unit symbol, and neither the word “degree” nor the degree symbol (°). The degree **Celsius** (°C) is also allowed in the SI system, with both the word “degree” and the degree symbol used for Celsius measurements. Celsius degrees are the same magnitude as those of kelvin, but the two scales place their zeros in different places. Water freezes at 273.15 K (0 °C) and boils at 373.15 K (100 °C) by definition, and normal human body temperature is approximately 310 K (37 °C). The conversion between these two units and the Fahrenheit scale will be discussed later in this chapter.

1.2.1.4: Time

The SI base unit of time is the **second** (s). Small and large time intervals can be expressed with the appropriate prefixes; for example, 3 microseconds = 0.000003 s = 3 x 10^{-6} and 5 megaseconds = 5,000,000 s = 5 x 10^{6} s. Alternatively, hours, days, and years can be used.

1.2.2: Derived SI Units

We can derive many units from the seven SI base units. For example, we can use the base unit of length to define a unit of volume, and the base units of mass and length to define a unit of density.

1.2.2.1: Volume

Volume is the measure of the amount of space occupied by an object. The standard SI unit of volume is defined by the base unit of length (Figure **1.2.3**). The standard volume is a cubic meter (m^3), a cube with an edge length of exactly one meter. To dispense a cubic meter of water, we could build a cubic box with edge lengths of exactly one meter. This box would hold a cubic meter of water or any other substance.

A more commonly used unit of volume is derived from the decimeter (0.1 m, or 10 cm). A cube with edge lengths of exactly one decimeter contains a volume of one cubic decimeter (dm^3). A liter (L) is the more common name for the cubic decimeter. One **liter**

is about 1.06 quarts.

A **cubic centimeter** (cm^3) is the volume of a cube with an edge length of exactly one centimeter. The abbreviation **cc** (for **c**ubic **c**entimeter) is often used by health professionals. A cubic centimeter is equivalent to a milliliter (mL) and is 1/1000 of a liter.

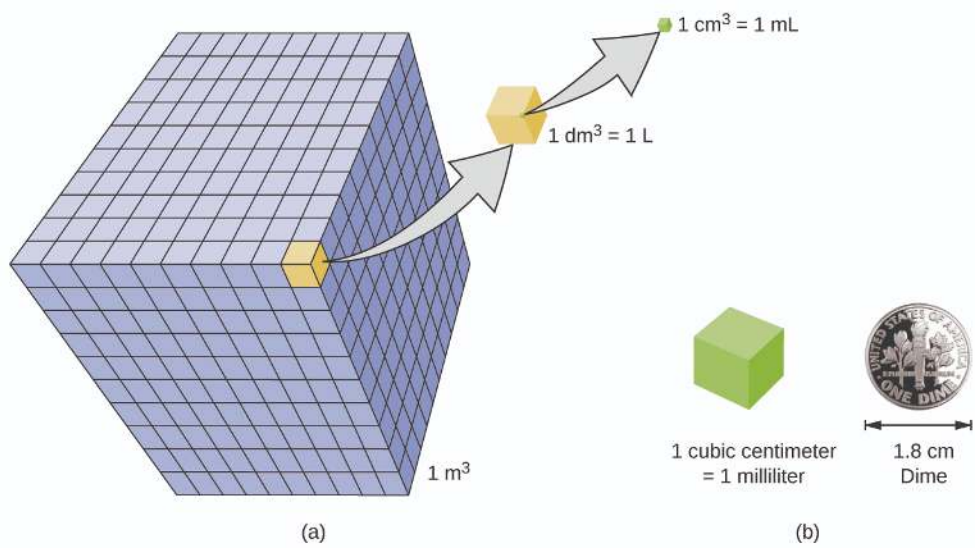


Figure **1.2.3**: (a) The relative volumes are shown for cubes of 1 m^3, 1 dm^3 (1 L), and 1 cm^3 (1 mL) (not to scale). (b) The diameter of a dime is compared relative to the edge length of a 1-cm^3 (1-mL) cube.

1.2.2.2: Density

We use the mass and volume of a substance to determine its density. Thus, the units of density are defined by the base units of mass and length.

The **density** of a substance is the ratio of the mass of a sample of the substance to its volume. The SI unit for density is the kilogram per cubic meter (kg/m^3). For many situations, however, this is an inconvenient unit, and we often use grams per cubic centimeter (g/cm^3) for the densities of solids and liquids, and grams per liter (g/L) for gases. Although there are exceptions, most liquids and solids have densities that range from about 0.7 g/cm^3 (the density of gasoline) to 19 g/cm^3 (the density of gold). The density of air is about 1.2 g/L. Table **1.2.3** shows the densities of some common substances.

Table **1.2.3**: Densities of Common Substances

Solids	Liquids	Gases (at 25 °C and 1 atm)
ice (at 0 °C) 0.92 g/cm^3	water 1.0 g/cm^3	dry air 1.20 g/L
oak (wood) 0.60–0.90 g/cm^3	ethanol 0.79 g/cm^3	oxygen 1.31 g/L
iron 7.9 g/cm^3	acetone 0.79 g/cm^3	nitrogen 1.14 g/L
copper 9.0 g/cm^3	glycerin 1.26 g/cm^3	carbon dioxide 1.80 g/L
lead 11.3 g/cm^3	olive oil 0.92 g/cm^3	helium 0.16 g/L
silver 10.5 g/cm^3	gasoline 0.70–0.77 g/cm^3	neon 0.83 g/L
gold 19.3 g/cm^3	mercury 13.6 g/cm^3	radon 9.1 g/L

While there are many ways to determine the density of an object, perhaps the most straightforward method involves separately finding the mass and volume of the object, and then dividing the mass of the sample by its volume. In the following example, the mass is found directly by weighing, but the volume is found indirectly through length measurements.

$$\text{density} = \frac{\text{mass}}{\text{volume}} \tag{1.2.1}$$

Example 1.2.1: Calculation of Density

Gold—in bricks, bars, and coins—has been a form of currency for centuries. In order to swindle people into paying for a brick of gold without actually investing in a brick of gold, people have considered filling the centers of hollow gold bricks with lead to fool buyers into thinking that the entire brick is gold. It does not work: Lead is a dense substance, but its density is not as great as that of gold, 19.3 g/cm^3. What is the density of lead if a cube of lead has an edge length of 2.00 cm and a mass of 90.7 g?

Solution

The density of a substance can be calculated by dividing its mass by its volume. The volume of a cube is calculated by cubing the edge length.

$$\text{volume of lead cube } = 2.00\ \text{cm} \times 2.00\ \text{cm} \times 2.00\ \text{cm} = 8.00\ \text{cm}^3$$

$$\text{density } = \frac{\text{mass}}{\text{volume}} = \frac{90.7\ \text{g}}{8.00\ \text{cm}^3} = 11.3\ \text{g/cm}^3$$

(We will discuss the reason for rounding to the first decimal place in the next section.)

Exercise 1.2.1

a. To three decimal places, what is the volume of a cube (cm^3) with an edge length of 0.843 cm?
b. If the cube in part (a) is copper and has a mass of 5.34 g, what is the density of copper to two decimal places?

Answer

a. 0.599 cm^3
b. 8.91 g/cm^3

Link to Learning

To learn more about the relationship between mass, volume, and density, use this interactive simulator to explore the density of different materials.

Example 1.2.2: Using Displacement of Water to Determine Density

This exercise uses a simulation to illustrate an alternative approach to the determination of density that involves measuring the object's volume via displacement of water. Use the simulator to determine the densities iron and wood.

Solution

Click the "turn fluid into water" button in the simulator to adjust the density of liquid in the beaker to 1.00 g/mL. Remove the red block from the beaker and note the volume of water is 25.5 mL. Select the iron sample by clicking "iron" in the table of materials at the bottom of the screen, place the iron block on the balance pan, and observe its mass is 31.48 g. Transfer the iron block to the beaker and notice that it sinks, displacing a volume of water equal to its own volume and causing the water level to rise to 29.5 mL. The volume of the iron block is therefore:

$$v_{\text{iron}} = 29.5mL - 25.5mL = 4.0mL$$

The density of the iron is then calculated to be:

$$\text{density } = \frac{\text{mass}}{\text{volume}} = \frac{31.48\ \text{g}}{4.0\ \text{mL}} = 7.9\ \text{g/mL}$$

Remove the iron block from the beaker, change the block material to wood, and then repeat the mass and volume measurements. Unlike iron, the wood block does not sink in the water but instead floats on the water's surface. To measure its volume, drag it beneath the water's surface so that it is fully submerged.

$$\text{density} = \frac{\text{mass}}{\text{volume}} = \frac{1.95\,\text{g}}{3.0\,\text{mL}} = 0.65\,\text{g/mL}$$

Note: The sink versus float behavior illustrated in this example demonstrates the property of “buoyancy”.

? Exercise 1.2.2

Following the water displacement approach, use the simulator to measure the density of the foam sample.

Answer

0.230 g/mL

1.2.3: Footnotes

- 1For details see https://www.nist.gov/pml/weights-and.../si-units-mass

---

This page titled 1.2: Units is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.4: Measurements** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

1.3: Matter

Learning Objectives

By the end of this section, you will be able to:

- Describe the basic properties of each physical state of matter: solid, liquid, and gas
- Distinguish between mass and weight
- Apply the law of conservation of matter
- Classify matter as an element, compound, homogeneous mixture, or heterogeneous mixture with regard to its physical state and composition
- Define and give examples of atoms and molecules

Matter is defined as anything that occupies space and has mass, and it is all around us. Solids and liquids are more obviously matter: We can see that they take up space, and their weight tells us that they have mass. Gases are also matter; if gases did not take up space, a balloon would not inflate (increase its volume) when filled with gas.

Solids, liquids, and gases are the three states of matter commonly found on earth (Figure **1.3.1**). A solid is rigid and possesses a definite shape. A liquid flows and takes the shape of its container, except that it forms a flat or slightly curved upper surface when acted upon by gravity. (In zero gravity, liquids assume a spherical shape.) Both liquid and solid samples have volumes that are very nearly independent of pressure. A gas takes both the shape and volume of its container.

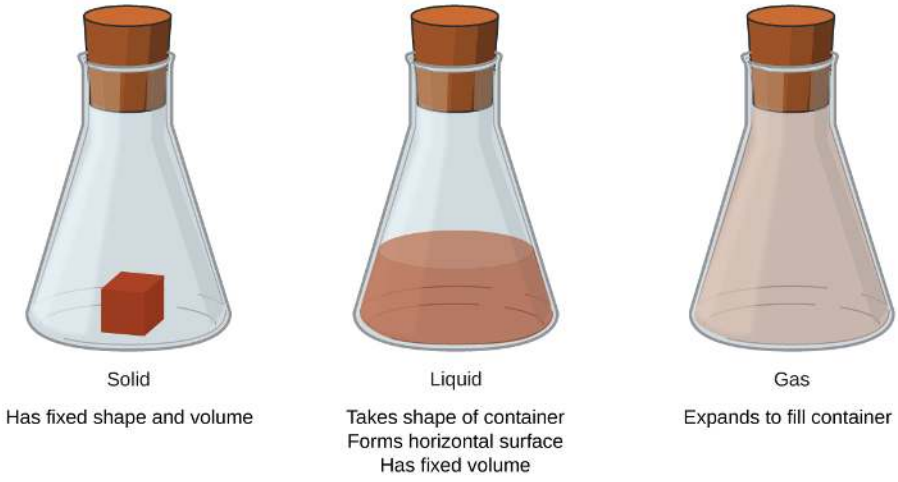


Figure **1.3.1**: The three most common states or phases of matter are solid, liquid, and gas.

A fourth state of matter, plasma, occurs naturally in the interiors of stars. A plasma is a gaseous state of matter that contains appreciable numbers of electrically charged particles (Figure **1.3.2**). The presence of these charged particles imparts unique properties to plasmas that justify their classification as a state of matter distinct from gases. In addition to stars, plasmas are found in some other high-temperature environments (both natural and man-made), such as lightning strikes, certain television screens, and specialized analytical instruments used to detect trace amounts of metals.



Figure **1.3.2**: A plasma torch can be used to cut metal. (credit: “Hypertherm”/Wikimedia Commons)

Link to Learning

In a tiny cell in a plasma television, the plasma emits ultraviolet light, which in turn causes the display at that location to appear a specific color. The composite of these tiny dots of color makes up the image that you see. Watch this video to learn more about plasma and the places you encounter it.

Some samples of matter appear to have properties of solids, liquids, and/or gases at the same time. This can occur when the sample is composed of many small pieces. For example, we can pour sand as if it were a liquid because it is composed of many small grains of solid sand. Matter can also have properties of more than one state when it is a mixture, such as with clouds. Clouds appear to behave somewhat like gases, but they are actually mixtures of air (gas) and tiny particles of water (liquid or solid).

The mass of an object is a measure of the amount of matter in it. One way to measure an object’s mass is to measure the force it takes to accelerate the object. It takes much more force to accelerate a car than a bicycle because the car has much more mass. A more common way to determine the mass of an object is to use a balance to compare its mass with a standard mass.

Although weight is related to mass, it is not the same thing. Weight refers to the force that gravity exerts on an object. This force is directly proportional to the mass of the object. The weight of an object changes as the force of gravity changes, but its mass does not. An astronaut’s mass does not change just because she goes to the moon. But her weight on the moon is only one-sixth her earth-bound weight because the moon’s gravity is only one-sixth that of the earth’s. She may feel “weightless” during her trip when she experiences negligible external forces (gravitational or any other), although she is, of course, never “massless.”

The law of conservation of matter summarizes many scientific observations about matter: It states that *there is no detectable change in the total quantity of matter present when matter converts from one type to another (a chemical change) or changes among solid, liquid, or gaseous states (a physical change)*. Brewing beer and the operation of batteries provide examples of the conservation of matter (Figure **1.3.3**). During the brewing of beer, the ingredients (water, yeast, grains, malt, hops, and sugar) are converted into beer (water, alcohol, carbonation, and flavoring substances) with no actual loss of substance. This is most clearly seen during the bottling process, when glucose turns into ethanol and carbon dioxide, and the total mass of the substances does not change. This can also be seen in a lead-acid car battery: The original substances (lead, lead oxide, and sulfuric acid), which are capable of producing electricity, are changed into other substances (lead sulfate and water) that do not produce electricity, with no change in the actual amount of matter.

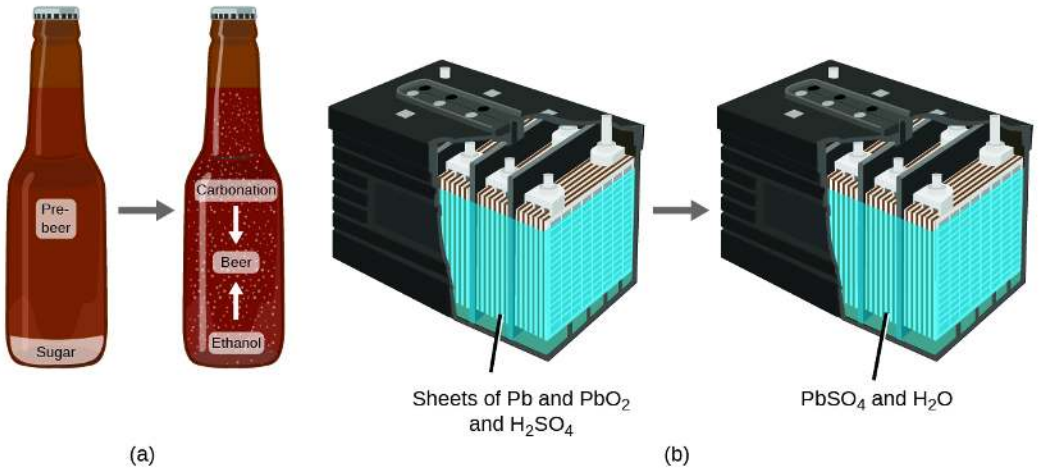


Figure **1.3.3**: (a) The mass of beer precursor materials is the same as the mass of beer produced: Sugar has become alcohol and carbon dioxide. (b) The mass of the lead, lead oxide, and sulfuric acid consumed by the production of electricity is exactly equal to the mass of lead sulfate and water that is formed.

Although this conservation law holds true for all conversions of matter, convincing examples are few and far between because, outside of the controlled conditions in a laboratory, we seldom collect all of the material that is produced during a particular conversion. For example, when you eat, digest, and assimilate food, all of the matter in the original food is preserved. But because some of the matter is incorporated into your body, and much is excreted as various types of waste, it is challenging to verify by measurement.

1.3.1: Classifying Matter

Matter can be classified into several categories. Two broad categories are mixtures and pure substances. A pure substance has a constant composition. All specimens of a pure substance have exactly the same makeup and properties. Any sample of sucrose (table sugar) consists of 42.1% carbon, 6.5% hydrogen, and 51.4% oxygen by mass. Any sample of sucrose also has the same physical properties, such as melting point, color, and sweetness, regardless of the source from which it is isolated.

Pure substances may be divided into two classes: elements and compounds. Pure substances that cannot be broken down into simpler substances by chemical changes are called elements. Iron, silver, gold, aluminum, sulfur, oxygen, and copper are familiar examples of the more than 100 known elements, of which about 90 occur naturally on the earth, and two dozen or so have been created in laboratories.

Pure substances that are comprised of two or more elements are called compounds. Compounds may be broken down by chemical changes to yield either elements or other compounds, or both. Mercury(II) oxide, an orange, crystalline solid, can be broken down by heat into the elements mercury and oxygen (Figure **1.3.4**). When heated in the absence of air, the compound sucrose is broken down into the element carbon and the compound water. (The initial stage of this process, when the sugar is turning brown, is known as caramelization—this is what imparts the characteristic sweet and nutty flavor to caramel apples, caramelized onions, and caramel). Silver(I) chloride is a white solid that can be broken down into its elements, silver and chlorine, by absorption of light. This property is the basis for the use of this compound in photographic films and photochromic eyeglasses (those with lenses that darken when exposed to light).

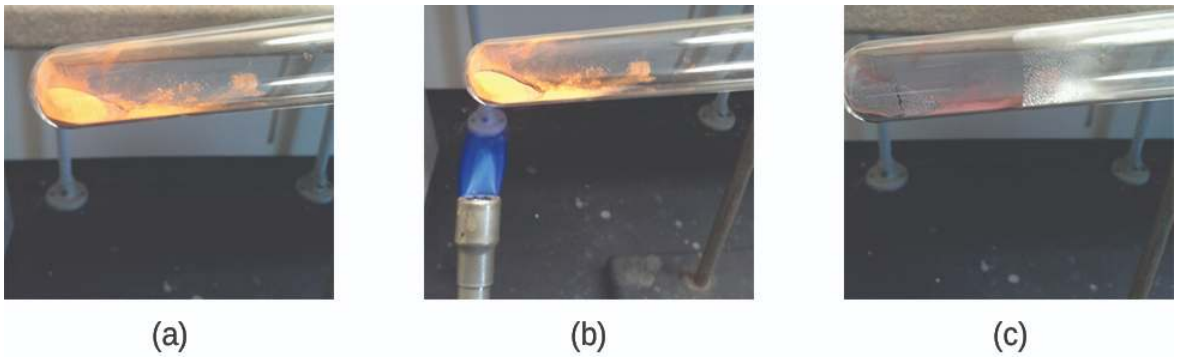


Figure **1.3.4**: (a) The compound mercury(II) oxide, (b) when heated, (c) decomposes into silvery droplets of liquid mercury and invisible oxygen gas. (credit: modification of work by Paul Flowers)

Link to Learning

Many compounds break down when heated. This site shows the breakdown of mercury oxide, HgO. You can also view an example of the photochemical decomposition of silver chloride (AgCl), the basis of early photography.

The properties of combined elements are different from those in the free, or uncombined, state. For example, white crystalline sugar (sucrose) is a compound resulting from the chemical combination of the element carbon, which is a black solid in one of its uncombined forms, and the two elements hydrogen and oxygen, which are colorless gases when uncombined. Free sodium, an element that is a soft, shiny, metallic solid, and free chlorine, an element that is a yellow-green gas, combine to form sodium chloride (table salt), a compound that is a white, crystalline solid.

A mixture is composed of two or more types of matter that can be present in varying amounts and can be separated by physical changes, such as evaporation (you will learn more about this later). A mixture with a composition that varies from point to point is called a heterogeneous mixture. Italian dressing is an example of a heterogeneous mixture (Figure **1.3.5**). Its composition can vary because it may be prepared from varying amounts of oil, vinegar, and herbs. It is not the same from point to point throughout the mixture—one drop may be mostly vinegar, whereas a different drop may be mostly oil or herbs because the oil and vinegar separate and the herbs settle. Other examples of heterogeneous mixtures are chocolate chip cookies (we can see the separate bits of chocolate, nuts, and cookie dough) and granite (we can see the quartz, mica, feldspar, and more).

A homogeneous mixture, also called a solution, exhibits a uniform composition and appears visually the same throughout. An example of a solution is a sports drink, consisting of water, sugar, coloring, flavoring, and electrolytes mixed together uniformly (Figure **1.3.5**). Each drop of a sports drink tastes the same because each drop contains the same amounts of water, sugar, and other components. Note that the composition of a sports drink can vary—it could be made with somewhat more or less sugar, flavoring, or other components, and still be a sports drink. Other examples of homogeneous mixtures include air, maple syrup, gasoline, and a solution of salt in water.



Figure **1.3.5**: (a) Oil and vinegar salad dressing is a heterogeneous mixture because its composition is not uniform throughout. (b) A commercial sports drink is a homogeneous mixture because its composition is uniform throughout. (credit a “left”: modification of work by John Mayer; credit a “right”: modification of work by Umberto Salvagnin; credit b “left: modification of work by Jeff Bedford)

Although there are just over 100 elements, tens of millions of chemical compounds result from different combinations of these elements. Each compound has a specific composition and possesses definite chemical and physical properties that distinguish it from all other compounds. And, of course, there are innumerable ways to combine elements and compounds to form different mixtures. A summary of how to distinguish between the various major classifications of matter is shown in (Figure **1.3.6**).

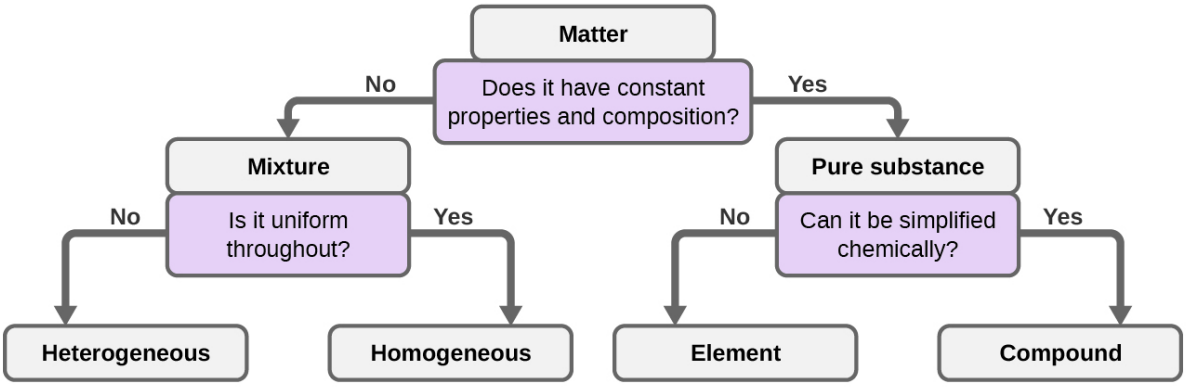


Figure **1.3.6**: Depending on its properties, a given substance can be classified as a homogeneous mixture, a heterogeneous mixture, a compound, or an element.

Eleven elements make up about 99% of the earth's crust and atmosphere (Table **1.3.1**). Oxygen constitutes nearly one-half and silicon about one-quarter of the total quantity of these elements. A majority of elements on earth are found in chemical combinations with other elements; about one-quarter of the elements are also found in the free state.

Table **1.3.1**: Elemental Composition of Earth

Element	Symbol	Percent Mass	Element	Symbol	Percent Mass
oxygen	O	49.20	chlorine	Cl	0.19
silicon	Si	25.67	phosphorus	P	0.11
aluminum	Al	7.50	manganese	Mn	0.09
iron	Fe	4.71	carbon	C	0.08
calcium	Ca	3.39	sulfur	S	0.06
sodium	Na	2.63	barium	Ba	0.04
potassium	K	2.40	nitrogen	N	0.03
magnesium	Mg	1.93	fluorine	F	0.03
hydrogen	H	0.87	strontium	Sr	0.02
titanium	Ti	0.58	all others	-	0.47

1.3.2: Atoms and Molecules

An atom is the smallest particle of an element that has the properties of that element and can enter into a chemical combination. Consider the element gold, for example. Imagine cutting a gold nugget in half, then cutting one of the halves in half, and repeating this process until a piece of gold remained that was so small that it could not be cut in half (regardless of how tiny your knife may be). This minimally sized piece of gold is an atom (from the Greek *atomos*, meaning "indivisible") (Figure **1.3.7**). This atom would no longer be gold if it were divided any further.

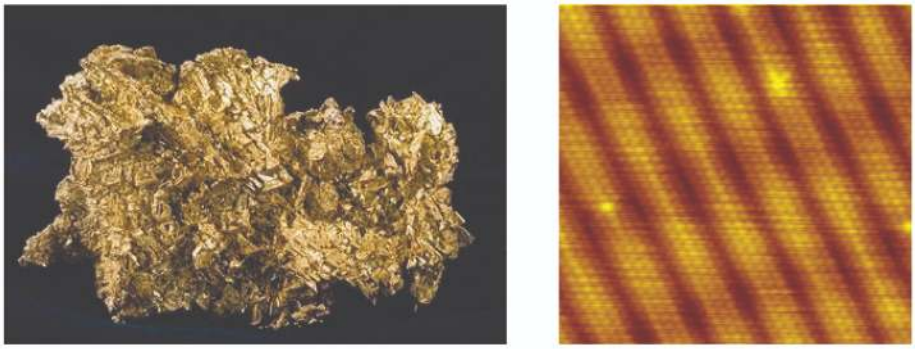


Figure **1.3.7**: (a) This photograph shows a gold nugget. (b) A scanning-tunneling microscope (STM) can generate views of the surfaces of solids, such as this image of a gold crystal. Each sphere represents one gold atom. (credit a: modification of work by United States Geological Survey; credit b: modification of work by "Erwinrossen"/Wikimedia Commons)

The first suggestion that matter is composed of atoms is attributed to the Greek philosophers Leucippus and Democritus, who developed their ideas in the 5th century BCE. However, it was not until the early nineteenth century that John Dalton (1766–1844), a British schoolteacher with a keen interest in science, supported this hypothesis with quantitative measurements. Since that time, repeated experiments have confirmed many aspects of this hypothesis, and it has become one of the central theories of chemistry. Other aspects of Dalton's atomic theory are still used but with minor revisions (details of Dalton's theory are provided in the chapter on atoms and molecules).

An atom is so small that its size is difficult to imagine. One of the smallest things we can see with our unaided eye is a single thread of a spider web: These strands are about 1/10,000 of a centimeter (0.0001 cm) in diameter. Although the cross-section of one strand is almost impossible to see without a microscope, it is huge on an atomic scale. A single carbon atom in the web has a diameter of about 0.000000015 centimeter, and it would take about 7000 carbon atoms to span the diameter of the strand. To put this in perspective, if a carbon atom were the size of a dime, the cross-section of one strand would be larger than a football field, which would require about 150 million carbon atom "dimes" to cover it. (Figure **1.3.8**) shows increasingly close microscopic and atomic-level views of ordinary cotton.

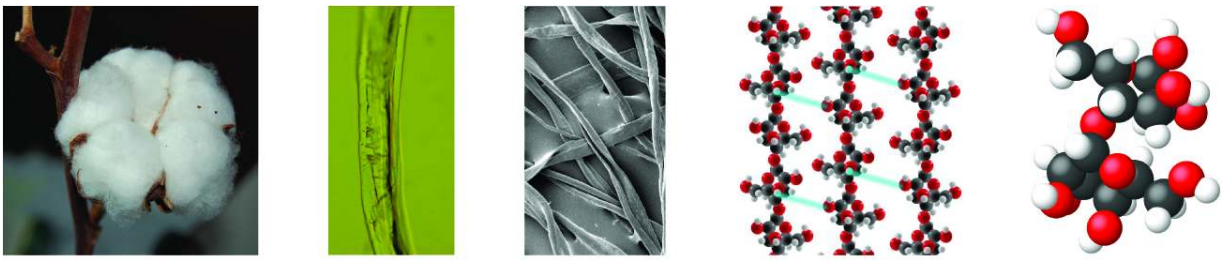


Figure **1.3.8**: These images provide an increasingly closer view: (a) a cotton boll, (b) a single cotton fiber viewed under an optical microscope (magnified 40 times), (c) an image of a cotton fiber obtained with an electron microscope (much higher magnification than with the optical microscope); and (d and e) atomic-level models of the fiber (spheres of different colors represent atoms of different elements). (credit c: modification of work by "Featheredtar"/Wikimedia Commons)

An atom is so light that its mass is also difficult to imagine. A billion lead atoms (1,000,000,000 atoms) weigh about $3\ 10^{-13}$ grams, a mass that is far too light to be weighed on even the world's most sensitive balances. It would require over 300,000,000,000,000 lead atoms (300 trillion, or $3\ 10^{14}$) to be weighed, and they would weigh only 0.0000001 gram.

It is rare to find collections of individual atoms. Only a few elements, such as the gases helium, neon, and argon, consist of a collection of individual atoms that move about independently of one another. Other elements, such as the gases hydrogen, nitrogen, oxygen, and chlorine, are composed of units that consist of pairs of atoms (Figure **1.3.9**). One form of the element phosphorus consists of units composed of four phosphorus atoms. The element sulfur exists in various forms, one of which consists of units composed of eight sulfur atoms. These units are called molecules. A molecule consists of two or more atoms joined by strong forces called chemical bonds. The atoms in a molecule move around as a unit, much like the cans of soda in a six-pack or a bunch of keys joined together on a single key ring. A molecule may consist of two or more identical atoms, as in the molecules found in

the elements hydrogen, oxygen, and sulfur, or it may consist of two or more different atoms, as in the molecules found in water. Each water molecule is a unit that contains two hydrogen atoms and one oxygen atom. Each glucose molecule is a unit that contains 6 carbon atoms, 12 hydrogen atoms, and 6 oxygen atoms. Like atoms, molecules are incredibly small and light. If an ordinary glass of water were enlarged to the size of the earth, the water molecules inside it would be about the size of golf balls.

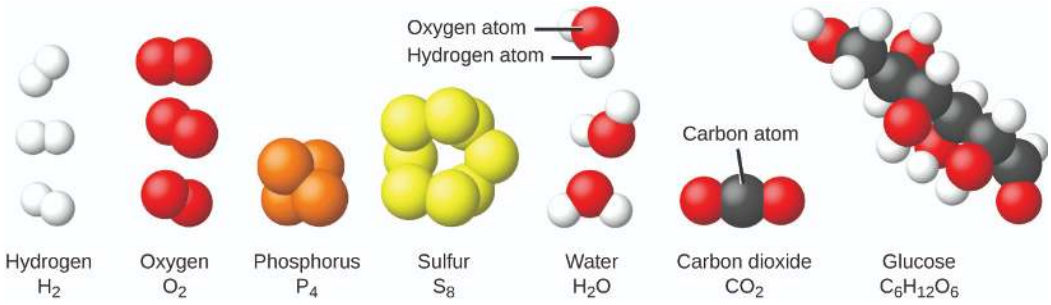


Figure **1.3.9**: The elements hydrogen, oxygen, phosphorus, and sulfur form molecules consisting of two or more atoms of the same element. The compounds water, carbon dioxide, and glucose consist of combinations of atoms of different elements.

Chemistry in Everyday Life: Decomposition of Water / Production of Hydrogen

Water consists of the elements hydrogen and oxygen combined in a 2 to 1 ratio. Water can be broken down into hydrogen and oxygen gases by the addition of energy. One way to do this is with a battery or power supply, as shown in (Figure **1.3.10**).

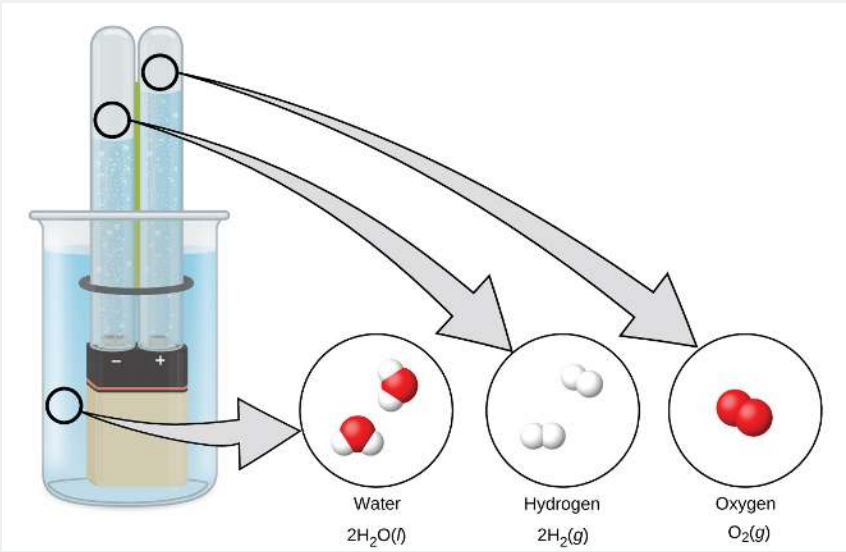


Figure **1.3.10**: The decomposition of water is shown at the macroscopic, microscopic, and symbolic levels. The battery provides an electric current (microscopic) that decomposes water. At the macroscopic level, the liquid separates into the gases hydrogen (on the left) and oxygen (on the right). Symbolically, this change is presented by showing how liquid H_2O separates into H_2 and O_2 gases.

The breakdown of water involves a rearrangement of the atoms in water molecules into different molecules, each composed of two hydrogen atoms and two oxygen atoms, respectively. Two water molecules form one oxygen molecule and two hydrogen molecules. The representation for what occurs, will be explored in more depth in later chapters.

The two gases produced have distinctly different properties. Oxygen is not flammable but is required for combustion of a fuel, and hydrogen is highly flammable and a potent energy source. How might this knowledge be applied in our world? One application involves research into more fuel-efficient transportation. Fuel-cell vehicles (FCV) run on hydrogen instead of gasoline (Figure **1.3.11**). They are more efficient than vehicles with internal combustion engines, are nonpolluting, and reduce greenhouse gas emissions, making us less dependent on fossil fuels. FCVs are not yet economically viable, however, and current hydrogen production depends on natural gas. If we can develop a process to economically decompose water, or produce hydrogen in another environmentally sound way, FCVs may be the way of the future.

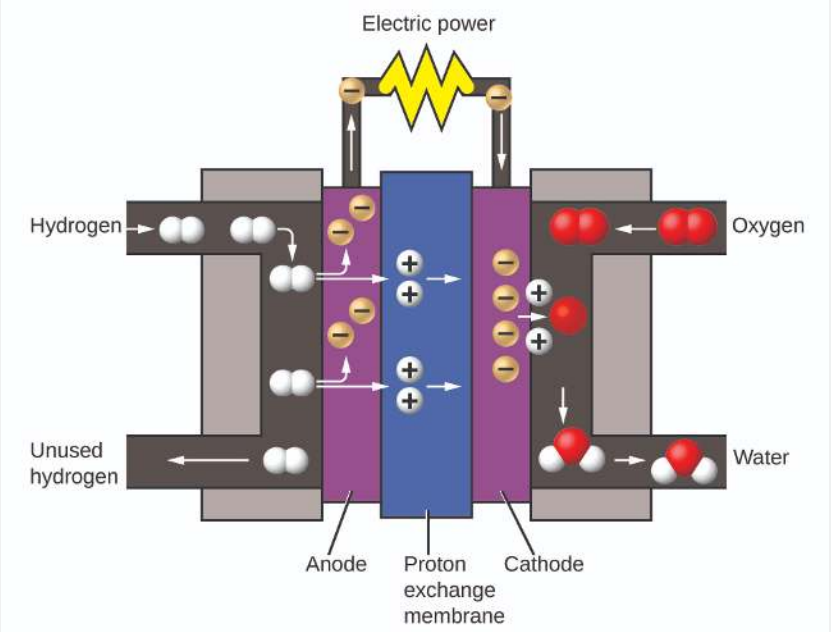


Figure **1.3.11**: A fuel cell generates electrical energy from hydrogen and oxygen via an electrochemical process and produces only water as the waste product.

Chemistry in Everyday Life: Chemistry of Cell Phones

Imagine how different your life would be without cell phones (Figure **1.3.12**) and other smart devices. Cell phones are made from numerous chemical substances, which are extracted, refined, purified, and assembled using an extensive and in-depth understanding of chemical principles. About 30% of the elements that are found in nature are found within a typical smart phone. The case/body/frame consists of a combination of sturdy, durable polymers composed primarily of carbon, hydrogen, oxygen, and nitrogen [acrylonitrile butadiene styrene (ABS) and polycarbonate thermoplastics], and light, strong, structural metals, such as aluminum, magnesium, and iron. The display screen is made from a specially toughened glass (silica glass strengthened by the addition of aluminum, sodium, and potassium) and coated with a material to make it conductive (such as indium tin oxide). The circuit board uses a semiconductor material (usually silicon); commonly used metals like copper, tin, silver, and gold; and more unfamiliar elements such as yttrium, praseodymium, and gadolinium. The battery relies upon lithium ions and a variety of other materials, including iron, cobalt, copper, polyethylene oxide, and polyacrylonitrile.

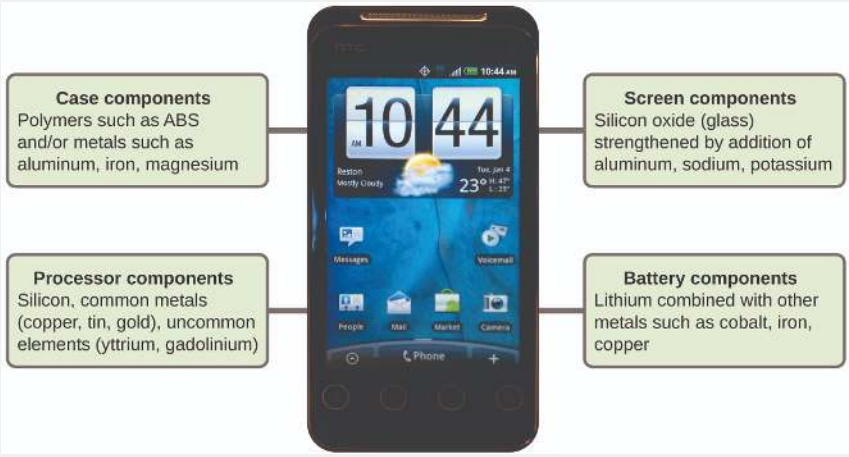


Figure **1.3.12**: Almost one-third of naturally occurring elements are used to make a cell phone. (credit: modification of work by John Taylor)

This page titled 1.3: Matter is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.2: Phases and Classification of Matter** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

1.4: Physical and Chemical Properties

Learning Objectives

By the end of this section, you will be able to

- Identify properties of and changes in matter as physical or chemical
- Identify properties of matter as extensive or intensive

The characteristics that distinguish one substance from another are called properties. A physical property is a characteristic of matter that is not associated with a change in its chemical composition. Familiar examples of physical properties include density, color, hardness, melting and boiling points, and electrical conductivity. Some physical properties, such as density and color, may be observed without changing the physical state of the matter. Other physical properties, such as the melting temperature of iron or the freezing temperature of water, can only be observed as matter undergoes a physical change. A physical change is a change in the state or properties of matter without any accompanying change in the chemical identities of the substances contained in the matter. Physical changes are observed when wax melts, when sugar dissolves in coffee, and when steam condenses into liquid water (Figure 1.18). Other examples of physical changes include magnetizing and demagnetizing metals (as is done with common antitheft security tags) and grinding solids into powders (which can sometimes yield noticeable changes in color). In each of these examples, there is a change in the physical state, form, or properties of the substance but no change in its chemical composition.



(a) (b)

Figure 1.18 (a) Wax undergoes a physical change when solid wax is heated and forms liquid wax. (b) Steam condensing inside a cooking pot is a physical change, as water vapor is changed into liquid water. (credit a: modification of work by "95jb14"/Wikimedia Commons; credit b: modification of work by "mjneuby"/Flickr)

The change of one type of matter into another type (or the inability to change) is a chemical property. Examples of chemical properties include flammability, toxicity, acidity, and many other types of reactivity. Iron, for example, combines with oxygen in the presence of water to form rust; chromium does not oxidize (Figure 1.19). Nitroglycerin is very dangerous because it explodes easily; neon poses almost no hazard because it is very unreactive.



(a) (b)

Figure 1.19 (a) One of the chemical properties of iron is that it rusts; (b) one of the chemical properties of chromium is that it does not. (credit a: modification of work by Tony Hisgett; credit b: modification of work by "Atoma"/Wikimedia Commons)

A chemical change always produces one or more types of matter that differ from the matter present before the change. The formation of rust is a chemical change because rust is a different kind of matter than the iron, oxygen, and water present before the rust formed. The explosion of nitroglycerin is a chemical change because the gases produced are very different kinds of matter from the original substance. Other examples of chemical changes include reactions that are performed in a lab (such as copper reacting with nitric acid), all forms of combustion (burning), and food being cooked, digested, or rotting (Figure 1.20).

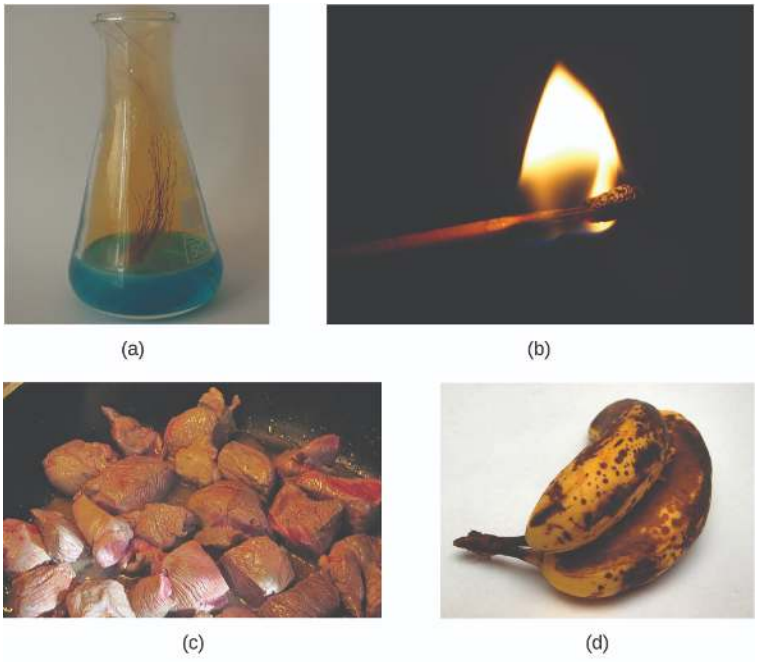


Figure 1.20 (a) Copper and nitric acid undergo a chemical change to form copper nitrate and brown, gaseous nitrogen dioxide. (b) During the combustion of a match, cellulose in the match and oxygen from the air undergo a chemical change to form carbon dioxide and water vapor. (c) Cooking red meat causes a number of chemical changes, including the oxidation of iron in myoglobin that results in the familiar red-to-brown color change. (d) A banana turning brown is a chemical change as new, darker (and less tasty) substances form. (credit b: modification of work by Jeff Turner; credit c: modification of work by Gloria Cabada-Leman; credit d: modification of work by Roberto Verzo)

Properties of matter fall into one of two categories. If the property depends on the amount of matter present, it is an extensive property. The mass and volume of a substance are examples of extensive properties; for instance, a gallon of milk has a larger mass than a cup of milk. The value of an extensive property is directly proportional to the amount of matter in question. If the property of a sample of matter does not depend on the amount of matter present, it is an intensive property. Temperature is an example of an intensive property. If the gallon and cup of milk are each at 20 °C (room temperature), when they are combined, the temperature remains at 20 °C. As another example, consider the distinct but related properties of heat and temperature. A drop of hot cooking oil spattered on your arm causes brief, minor discomfort, whereas a pot of hot oil yields severe burns. Both the drop and the pot of oil are at the same temperature (an intensive property), but the pot clearly contains much more heat (an extensive property).

Chemistry in Everyday Life

1.4.0.1: Hazard Diamond

You may have seen the symbol shown in Figure 1.21 on containers of chemicals in a laboratory or workplace. Sometimes called a “fire diamond” or “hazard diamond,” this chemical hazard diamond provides valuable information that briefly summarizes the various dangers of which to be aware when working with a particular substance.

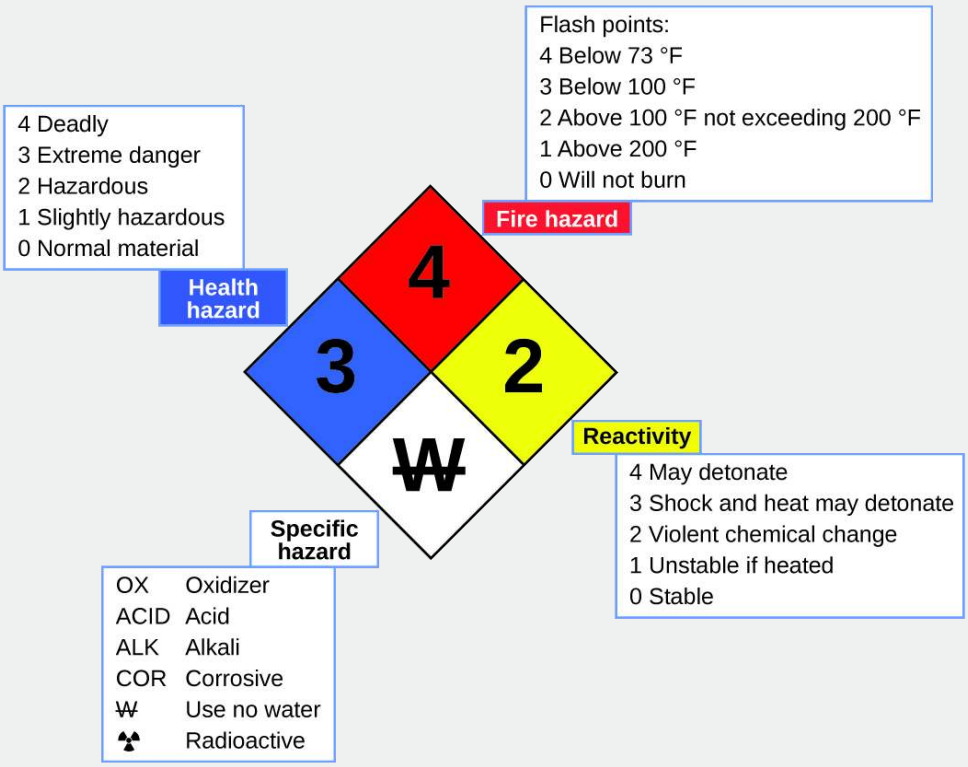


Figure 1.21 The National Fire Protection Agency (NFPA) hazard diamond summarizes the major hazards of a chemical substance.

The National Fire Protection Agency (NFPA) 704 Hazard Identification System was developed by NFPA to provide safety information about certain substances. The system details flammability, reactivity, health, and other hazards. Within the overall diamond symbol, the top (red) diamond specifies the level of fire hazard (temperature range for flash point). The blue (left) diamond indicates the level of health hazard. The yellow (right) diamond describes reactivity hazards, such as how readily the substance will undergo detonation or a violent chemical change. The white (bottom) diamond points out special hazards, such as if it is an oxidizer (which allows the substance to burn in the absence of air/oxygen), undergoes an unusual or dangerous reaction with water, is corrosive, acidic, alkaline, a biological hazard, radioactive, and so on. Each hazard is rated on a scale from 0 to 4, with 0 being no hazard and 4 being extremely hazardous.

While many elements differ dramatically in their chemical and physical properties, some elements have similar properties. For example, many elements conduct heat and electricity well, whereas others are poor conductors. These properties can be used to sort the elements into three classes: metals (elements that conduct well), nonmetals (elements that conduct poorly), and metalloids (elements that have intermediate conductivities).

The periodic table is a table of elements that places elements with similar properties close together (Figure 1.22). You will learn more about the periodic table as you continue your study of chemistry.

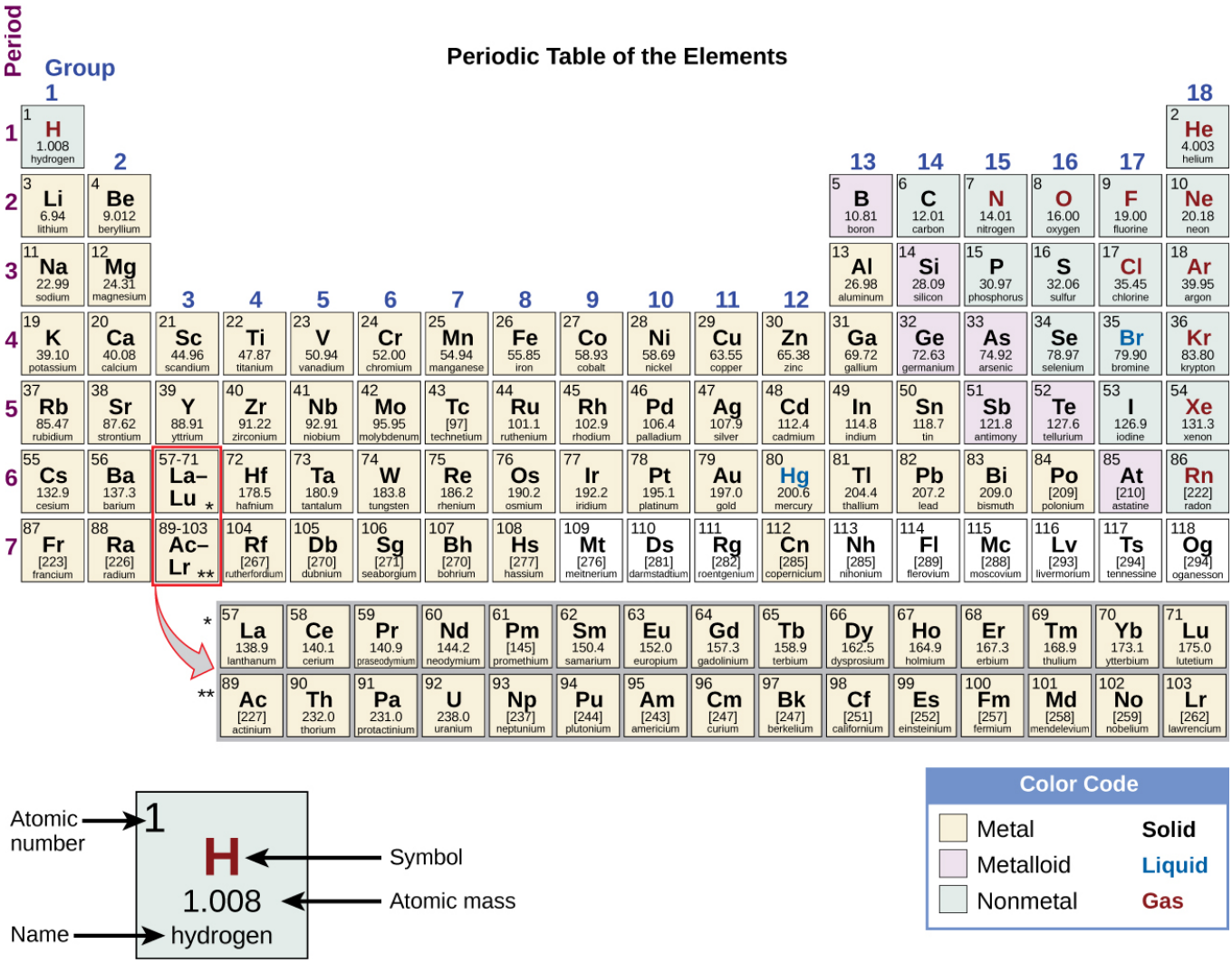


Figure 1.22 The periodic table shows how elements may be grouped according to certain similar properties. Note the background color denotes whether an element is a metal, metalloid, or nonmetal, whereas the element symbol color indicates whether it is a solid, liquid, or gas.

This page titled 1.4: Physical and Chemical Properties is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

1.5: Case Study- Using the Scientific Method to Diagnose an Autoimmune Disorder

Patient Information:

- Patient Name: Emily
- Age: 32
- Gender: Female
- Symptoms: Fatigue, joint pain, muscle weakness, skin rash, hair loss, sensitivity to cold

Introduction: Emily, a 32-year-old female, presented with a complex set of symptoms including fatigue, joint pain, muscle weakness, skin rash, hair loss, and sensitivity to cold. These symptoms suggested a potential autoimmune disorder. To accurately diagnose the condition, a systematic approach based on the scientific method was employed.

Step 1: Observation and Background Research: Emily's primary care physician observed her symptoms and medical history. Initial research was conducted to gather information about potential autoimmune disorders that matched her symptoms. Given the combination of her symptoms, conditions such as lupus, rheumatoid arthritis, and Hashimoto's thyroiditis were considered.

Step 2: Formulating Hypotheses: Based on the initial observation and background research, two primary hypotheses were formulated:

1. Hypothesis A: Emily may have systemic lupus erythematosus (SLE), given the presence of skin rash, joint pain, and fatigue, which are common symptoms of this autoimmune disorder.
2. Hypothesis B: Emily could be suffering from Hashimoto's thyroiditis as hair loss, fatigue, and sensitivity to cold are consistent with this disorder affecting the thyroid gland.

Step 3: Designing Experiments: To test the hypotheses, a series of diagnostic tests were designed and performed:

1. Blood Tests: A comprehensive blood panel was conducted to assess markers of inflammation (e.g., C-reactive protein), autoimmune antibodies (e.g., antinuclear antibodies for lupus), and thyroid function (e.g., TSH, T3, T4).
2. Skin Biopsy: A skin biopsy was performed to examine the rash histologically and assess the presence of specific immune cells.
3. Joint Imaging: X-rays and/or MRI scans were conducted to examine joint health and detect any inflammation or damage.
4. Clinical Assessment: Detailed physical examinations were performed to evaluate joint mobility, muscle strength, and overall health.

Step 4: Data Collection and Analysis: The test results indicated elevated levels of antinuclear antibodies, along with characteristic histological findings in the skin biopsy consistent with lupus. The blood panel also showed thyroid dysfunction, including elevated TSH levels and reduced T3 and T4 levels, confirming Hashimoto's thyroiditis. Joint imaging revealed signs of inflammation in several joints.

Step 5: Drawing Conclusions: The combination of elevated antinuclear antibodies, skin biopsy results, thyroid dysfunction, and joint inflammation supported the following conclusions:

1. Emily was diagnosed with systemic lupus erythematosus (SLE) based on the presence of specific antibodies, skin rash, and joint inflammation.
2. She was also diagnosed with Hashimoto's thyroiditis due to thyroid dysfunction and sensitivity to cold.

Step 6: Communication: The diagnoses were communicated to Emily, along with explanations of each condition, potential treatment options, and the need for ongoing monitoring and management.

Step 7: Further Testing and Treatment: Further tests, such as kidney function assessments (lupus nephritis evaluation) and specific antibody panels, were conducted to evaluate the extent of organ involvement in lupus. Treatment plans were developed, including corticosteroids for symptom relief and disease-modifying antirheumatic drugs (DMARDs) for long-term management of both conditions. Collaboration with specialists such as rheumatologists and endocrinologists was initiated to ensure comprehensive care.

Case Study Questions:

1. What are the steps of the scientific method?
2. How can the Nursing Process be integrated into diagnosing and treating patients?

Hands-On Classroom Activity:

1. **Role-play:** After discussing these questions, students will participate in a role-playing activity that mirrors a medical case conference. They will apply the scientific method to analyze a fictitious patient's condition and suggest appropriate treatments. This interactive classroom exercise gives students a practical perspective on diagnosing and treating complex conditions such as autoimmune disorders, fostering a deeper comprehension of collaborative patient care.

Conclusion: In this case study, the scientific method was instrumental in accurately diagnosing Emily's complex presentation of symptoms as both systemic lupus erythematosus (SLE) and Hashimoto's thyroiditis. The systematic approach involving observation, hypothesis formulation, experimentation, data analysis, and drawing conclusions led to appropriate treatment strategies and a comprehensive understanding of her autoimmune disorders.

1.5: Case Study- Using the Scientific Method to Diagnose an Autoimmune Disorder is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

1.E: Exercises

Multiple-Choice Questions

1. Which of the following statements is false?
    a. A law explains why something is true.
    b. A law describes a series of experimental observations.
    c. A theory can be refuted by new experimental results.
    d. Unlike a hypothesis, experimental data is required to formulate a theory.
2. Which is a base unit of the SI system?
    a. Gram
    b. Liter
    c. Cubic centimeter
    d. Second
3. Which is a derived unit of the SI system?
    a. Kelvin
    b. Meter
    c. Milliliter
    d. Kilogram
4. You measure the mass of a 1 kg object five times: 0.978 kg, 0.979 kg, 0.979 kg, 0.976 kg, 0.977 kg. Are your results...?
    a. Accurate, but not precise
    b. Precise, but not accurate
    c. Both accurate and precise
    d. Neither accurate nor precise
5. Which quantity is exact?
    a. The number of eggs in a dozen
    b. The height of a person
    c. The mass of a dog
    d. The length of a table
6. Report the volume of the liquid in the graduated cylinder shown in the image to the right using the correct number of significant figures.



    a. 20 mL
    b. 19.7 mL
    c. 20.5 mL
    d. 19.75 mL
7. Which number has only 2 significant figures?
    a. 1082
    b. 0.94

c. 0.207

d. 6.23

8. What is the assumed uncertainty in the value 7.934 g?

   a. ±1 g

   b. ±0.1 g

   c. ±0.01 g

   d. ±0.001 g

9. Which of the following is an example of a homogeneous mixture?

   a. Air

   b. Chocolate chip ice cream

   c. Dirt

   d. Concrete

10. Which of the following is a mixture?

    a. Helium

    b. Copper

    c. Brass

    d. Iron

Warmup Problems

1. Write the following values in scientific notation:

   a. 0.000000025

   b. 4468241

2. Write the following values in scientific notation:

   a. 0.000091

   b. 3452

3. Rewrite the provided value using an appropriate SI prefix:

   a. 1342 m

   b. 0.00358 s

4. Rewrite the provided value using an appropriate SI prefix:

   a. 532000000 g

   b. 0.0000000081 L

5. How many significant figures are in each of the following values?

   a. 1.080

   b. 0.00034

6. How many significant figures are in each of the following values?

   a. 77.0

   b. 0.000005

7. Round the following values to three significant figures. Use scientific notation when appropriate.

a. 81372

b. 0.0234803

8. Round the following values to two significant figures. Use scientific notation when appropriate.

a. 5527

b. 0.0002025

9. Is wine an example of a mixture or a pure substance? Explain your reasoning.

10. Is water an example of a mixture or a pure substance? Explain your reasoning.

11. Is seawater an example of a heterogeneous or a homogeneous mixture? Explain your reasoning.

12. Is steel an example of a heterogeneous or a homogeneous mixture? Explain your reasoning.

Problems

1. Round the following value to two significant figures and express it using an appropriate prefix: 0.00389 g
2. Round the following value to three significant figures and express it using an appropriate prefix: 72918 m
3. Report the final answer to the correct number of significant figures: 3.06 + 5.3
4. Report the final answer to the correct number of significant figures: 10.83/3.75
5. Temperature conversion: The average temperature of a healthy human is 98.6 °F. Convert this value to degrees Celsius.
6. Temperature conversion: Isopropanol is often used as a disinfectant for injection sites on the body. It has a boiling point of 82.3 °C. What is the boiling point in degrees Fahrenheit?
7. Conservation of mass: When sucrose is burned in oxygen, it produces carbon dioxide and water. If 10.0 g of sucrose is burned in the presence of 11.2 g of oxygen and produces 15.4 g of carbon dioxide, what mass of water is produced?
8. Conservation of mass: If pure iron is exposed to oxygen in a moist environment, it forms iron(III) oxide, otherwise known as rust. This chemical reaction is an example of corrosion. How many grams of oxygen are needed if 24.7 g of iron is completely corroded to form 35.3 g of rust?

Challenge Problems

1. Report the final answer to the correct number of significant figures: (1034.3/22.8) - 5.66
2. Report the final answer to the correct number of significant figures: (6.311 × 5.82) + 1.04
3. The total mass of exactly 250 aspirin tablets was measured to be 81.25 g. What is the mass of a single aspirin tablet? Report your answer using an appropriate prefix.
4. Three solutions of volumes 34.6 mL, 20.004 mL, and 73.52 mL are combined to make one solution. What is the final volume of the solution? Express your answer using an appropriate prefix.

Health-Related Problems

1. Which has the smallest mass of pain medication, 25 mcg of fentanyl, 15 mg of morphine, or 0.200 g of ibuprofen? Convert them all to the same unit to compare.
2. Which has the smaller mass of heart medication, 40 mg of atorvastatin, 0.100 g of metoprolol, or 500 mg of warfarin? Convert them all to the same unit to compare.
3. Celsius is often used outside of the US for body temperature values. If a person has a temperature of 98.2 °F, what would it be in Celsius? What would it be for a fever of 100.8 °F?
4. Celsius is often used outside of the US for body temperature values. If a person has a temperature of 97.6 °F, what would it be in Celsius? What would it be for a hypothermic patient with a temperature of 94.5 °F?
5. If blood is allowed to settle or is centrifuged, the red blood cells and the clear plasma can be separated. Is blood a homogeneous or heterogeneous mixture?
6. Cloudy urine can be a sign of kidney problems or dehydration. If allowed to sit, the solids will settle out. Is cloudy urine a homogeneous or heterogeneous mixture?

1.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

2: Atoms and Elements

Learning Objectives

- Outline the historical development of chemistry
- Provide examples of the importance of chemistry in everyday life
- Describe the scientific method that informs the scientific process
- Differentiate among hypotheses, theories, and laws
- Provide examples illustrating macroscopic, microscopic, and symbolic domains

Throughout human history, people have tried to convert matter into more useful forms. Our Stone Age ancestors chipped pieces of flint into useful tools and carved wood into statues and toys. These endeavors involved changing the shape of a substance without changing the substance itself. But as our knowledge increased, humans began to change the composition of the substances as well—clay was converted into pottery, hides were cured to make garments, copper ores were transformed into copper tools and weapons, and grain was made into bread.

Humans began to practice chemistry when they learned to control fire and use it for cooking, making pottery, and smelting metals. Subsequently, they began to separate and use specific components of matter. A variety of drugs, such as aloe, myrrh, and opium, were isolated from plants. Dyes, such as indigo and Tyrian purple, were extracted from plant and animal matter. Metals were combined to form alloys—for example, copper and tin were mixed together to make bronze—and more elaborate smelting techniques produced iron. Alkalis were extracted from ashes, and soaps were prepared by combining these alkalis with fats. Alcohol was produced by fermentation and purified by distillation.

Attempts to understand the behavior of matter extend back more than 2500 years. As early as the sixth century BC, Greek philosophers discussed a system in which water was the basis of all things. You may have heard of the Greek postulate that matter consists of four elements: earth, air, fire, and water. Subsequently, an amalgamation of chemical technologies and philosophical speculations was spread from Egypt, China, and the eastern Mediterranean by alchemists, who endeavored to transform “base metals” such as lead into “noble metals” like gold and to create elixirs to cure disease and extend life (Figure **2.1**).



Figure **2.1**: This portrayal shows an alchemist’s workshop circa 1580. Although alchemy made some useful contributions to how to manipulate matter, it was not scientific by modern standards. (credit: Chemical Heritage Foundation).

A sketch depicts 4 people stirring and handling chemicals. The chemicals are held in a variety of barrels and large cylinders. Several of the containers are being heated over burning embers. A large stove in the laboratory is filled with burning embers. There is also a large chest in the corner that is producing steam.

From alchemy came the historical progressions that led to modern chemistry: the isolation of drugs from natural sources, metallurgy, and the dye industry. Today, chemistry continues to deepen our understanding and improve our ability to harness and

control the behavior of matter. This effort has been so successful that many people do not realize either the central position of chemistry among the sciences or the importance and universality of chemistry in daily life.

2.1: Chemistry: The Central Science

Chemistry is sometimes referred to as “the central science” for its interconnectedness with a vast array of other STEM disciplines (STEM stands for areas of study in the science, technology, engineering, and math fields). Chemistry and the language of chemists play vital roles in biology, medicine, materials science, forensics, environmental science, and many other fields (Figure **2.2**). The basic principles of physics are essential for understanding many aspects of chemistry, and there is extensive overlap between many subdisciplines within the two fields, such as chemical physics and nuclear chemistry. Mathematics, computer science, and information theory provide important tools that help us calculate, interpret, describe, and generally make sense of the chemical world. Biology and chemistry converge in biochemistry, which is crucial to understanding the many complex factors and processes that keep living organisms (such as us) alive. Chemical engineering, materials science, and nanotechnology combine chemical principles and empirical findings to produce useful substances, ranging from gasoline to fabrics to electronics. Agriculture, food science, veterinary science, brewing, and wine-making help provide sustenance in the form of food and drink to the world’s population. Medicine, pharmacology, biotechnology, and botany identify and produce substances that help keep us healthy. Environmental science, geology, oceanography, and atmospheric science incorporate many chemical ideas to help us better understand and protect our physical world. Chemical ideas are used to help understand the universe in astronomy and cosmology.

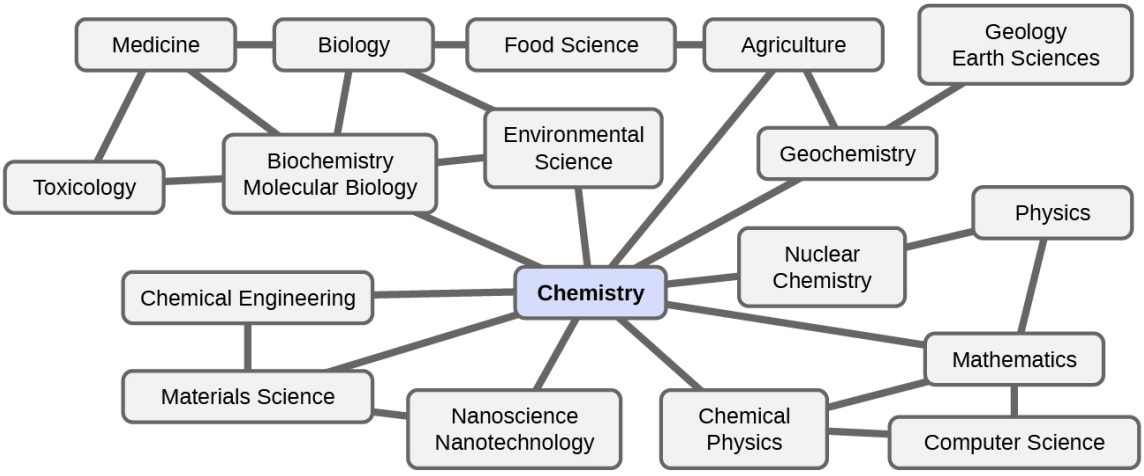


Figure **2.2**: Knowledge of chemistry is central to understanding a wide range of scientific disciplines. This diagram shows just some of the interrelationships between chemistry and other fields.

A flowchart shows a box containing chemistry at its center. Chemistry is connected to geochemistry, nuclear chemistry, chemical physics, nanoscience and nanotechnology, materials science, chemical engineering, biochemistry and molecular biology, environmental science, agriculture, and mathematics. Each of these disciplines is further connected to other related fields, including medicine, biology, food science, geology, earth sciences, toxicology, physics, and computer science.

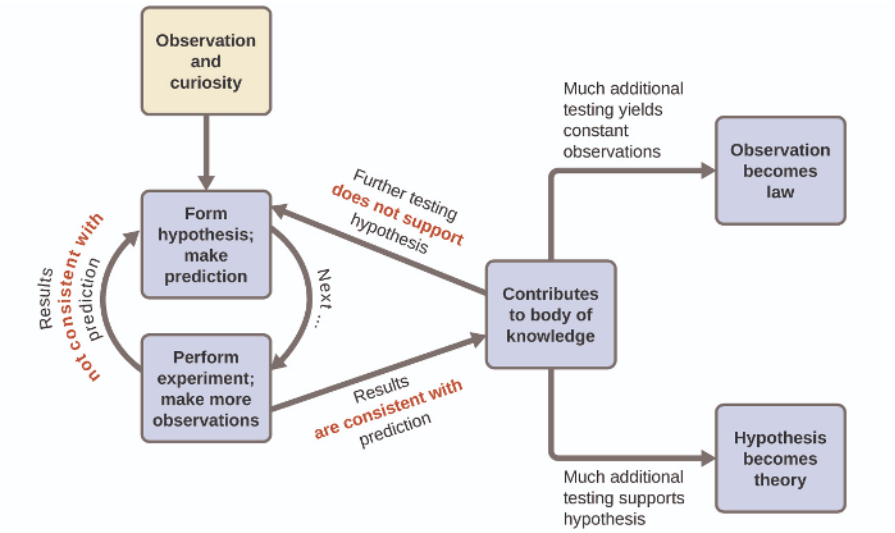
What are some changes in matter that are essential to daily life? Digesting and assimilating food, synthesizing polymers that are used to make clothing, containers, cookware, and credit cards, and refining crude oil into gasoline and other products are just a few examples. As you proceed through this course, you will discover many different examples of changes in the composition and structure of matter, how to classify these changes and how they occurred, their causes, the changes in energy that accompany them, and the principles and laws involved. As you learn about these things, you will be learning chemistry—the study of the composition, properties, and interactions of matter. The practice of chemistry is not limited to chemistry books or laboratories: It happens whenever someone is involved in changes in matter or in conditions that may lead to such changes.

2.2: The Scientific Method

Chemistry is a science based on observation and experimentation. Doing chemistry involves attempting to answer questions and explain observations in terms of the laws and theories of chemistry, using procedures that are accepted by the scientific community. There is no single route to answering a question or explaining an observation, but there is an aspect common to every approach: each uses knowledge based on experiments that can be reproduced to verify the results. Some routes involve a hypothesis, a

tentative explanation of observations that acts as a guide for gathering and checking information. We test a hypothesis by experimentation, calculation, and/or comparison with the experiments of others and then refine it as needed.

Some hypotheses are attempts to explain the behavior that is summarized in laws. The laws of science summarize a vast number of experimental observations and describe or predict some facet of the natural world. If such a hypothesis turns out to be capable of explaining a large body of experimental data, it can reach the status of a theory. Scientific theories are well substantiated, comprehensive, testable explanations of particular aspects of nature. Theories are accepted because they provide satisfactory explanations, but they can be modified if new data become available. The path of discovery that leads from question and observation to law or hypothesis to theory, combined with experimental verification of the hypothesis and any necessary modification of the theory, is called the scientific method (Figure **2.3**).



In this flowchart, the observation and curiosity box has an arrow pointing to a box labeled form hypothesis; make prediction. A curved arrow labeled next connects this box to a box labeled perform experiment; make more observations. Another arrow points back to the box that says form hypothesis; make prediction. This arrow is labeled results not consistent with prediction. Another arrow, labeled results are consistent with prediction points from the perform experiment box to a box labeled contributes to body of knowledge. However, an arrow also points from contributes to body of knowledge back to the form hypothesis; make prediction box. This arrow is labeled further testing does not support hypothesis. There are also two other arrows leading out from contributes to body of knowledge. One arrow is labeled much additional testing yields constant observations. This leads to the observation becomes law box. The other arrow is labeled much additional testing supports hypothesis. This arrow leads to the hypothesis becomes theory box.

Figure **2.3**: The scientific method follows a process similar to the one shown in this diagram. All the key components are shown, in roughly the right order. Scientific progress is seldom neat and clean: It requires open inquiry and the reworking of questions and ideas in response to findings.

2.3: The Domains of Chemistry

Chemists study and describe the behavior of matter and energy in three different domains: macroscopic, microscopic, and symbolic. These domains provide different ways of considering and describing chemical behavior.

Macro is a Greek word that means “large.” The macroscopic domain is familiar to us: it is the realm of everyday things that are large enough to be sensed directly by human sight or touch. In daily life, this includes the food you eat and the breeze you feel on your face. The macroscopic domain includes everyday and laboratory chemistry, where we observe and measure physical and chemical properties or changes such as density, solubility, and flammability.

The microscopic domain of chemistry is almost always visited in the imagination. *Micro* also comes from Greek and means “small.” Some aspects of the microscopic domains are visible through a microscope, such as a magnified image of graphite or bacteria. Viruses, for instance, are too small to be seen with the naked eye, but when we’re suffering from a cold, we’re reminded of how real they are.

However, most of the subjects in the microscopic domain of chemistry—such as atoms and molecules—are too small to be seen even with standard microscopes and often must be pictured in the mind. Other components of the microscopic domain include ions

and electrons, protons and neutrons, and chemical bonds, each of which is far too small to see. This domain includes the individual metal atoms in a wire, the ions that compose a salt crystal, the changes in individual molecules that result in a color change, the conversion of nutrient molecules into tissue and energy, and the evolution of heat as bonds that hold atoms together are created.

The symbolic domain contains the specialized language used to represent components of the macroscopic and microscopic domains. Chemical symbols (such as those used in the periodic table), chemical formulas, and chemical equations are part of the symbolic domain, as are graphs and drawings. We can also consider calculations as part of the symbolic domain. These symbols play an important role in chemistry because they help interpret the behavior of the macroscopic domain in terms of the components of the microscopic domain. One challenge for students learning chemistry is recognizing that the same symbols can represent different things in the macroscopic and microscopic domains, and one of the features that makes chemistry fascinating is the use of a domain that must be imagined to explain behavior in a domain that can be observed.

A helpful way to understand the three domains is via the essential and ubiquitous substance of water. That water is a liquid at moderate temperatures, will freeze to form a solid at lower temperatures, and boil to form a gas at higher temperatures (Figure 1.1.4) are macroscopic observations. But some properties of water fall into the microscopic domain—what we cannot observe with the naked eye. The description of water as comprising two hydrogen atoms and one oxygen atom, and the explanation of freezing and boiling in terms of attractions between these molecules, is within the microscopic arena. The formula H_2O, which can describe water at either the macroscopic or microscopic levels, is an example of the symbolic domain. The abbreviations (*g*) for gas, (*s*) for solid, and (*l*) for liquid are also symbolic.

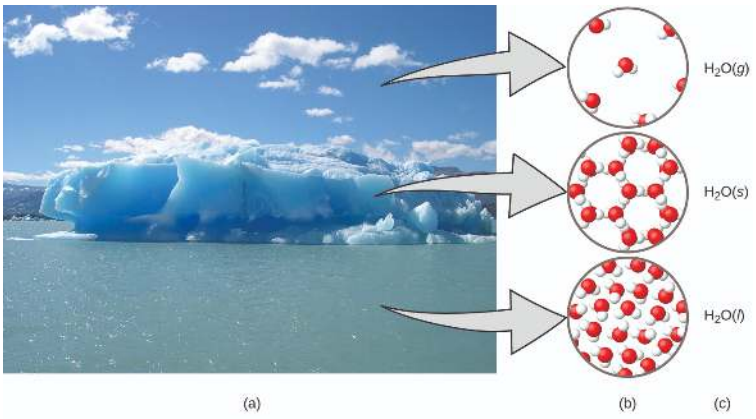


Figure **2.4**: (a) Moisture in the air, icebergs, and the ocean represent water in the macroscopic domain. (b) At the molecular level (microscopic domain), gas molecules are far apart and disorganized, solid water molecules are close together and organized, and liquid molecules are close together and disorganized. (c) The formula H_2O symbolizes water, and (g), (s), and (l) symbolize its phases. Note that clouds are actually comprised of either very small liquid water droplets or solid water crystals; gaseous water in our atmosphere is not visible to the naked eye, although it may be sensed as humidity. (credit a: modification of work by "Gorkaazk"/Wikimedia Commons).

Figure A shows a photo of an iceberg floating in a sea that has three arrows. Each arrow points to Figure B, which contains three diagrams showing how the water molecules are organized in the air, ice, and sea. In the air, which contains the gaseous form of water, H subscript 2 O gas, the water molecules are disconnected and widely spaced. In the ice, which is the solid form of water, H subscript 2 O solid, the water molecules are bonded together into rings, with each ring containing six water molecules. Three of these rings are connected to each other. In the sea, which is the liquid form of water, H subscript 2 O liquid, the water molecules are very densely packed. The molecules are not bonded together.

2.4: Key Concepts and Summary

Chemistry deals with the composition, structure, and properties of matter, and the ways by which various forms of matter may be interconverted. Thus, it occupies a central place in the study and practice of science and technology. Chemists use the scientific method to perform experiments, pose hypotheses, formulate laws, and develop theories so that they can better understand the behavior of the natural world. To do so, they operate in the macroscopic, microscopic, and symbolic domains. Chemists measure, analyze, purify, and synthesize a wide variety of substances that are important to our lives.

Glossary

chemistry
study of the composition, properties, and interactions of matter

hypothesis
tentative explanation of observations that acts as a guide for gathering and checking information

law
statement that summarizes a vast number of experimental observations, and describes or predicts some aspect of the natural world

macroscopic domain
realm of everyday things that are large enough to sense directly by human sight and touch

microscopic domain
realm of things that are much too small to be sensed directly

scientific method
path of discovery that leads from question and observation to law or hypothesis to theory, combined with experimental verification of the hypothesis and any necessary modification of the theory

symbolic domain
specialized language used to represent components of the macroscopic and microscopic domains, such as chemical symbols, chemical formulas, chemical equations, graphs, drawings, and calculations

theory
well-substantiated, comprehensive, testable explanation of a particular aspect of nature

---

This page titled 2: Atoms and Elements is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.1: Chemistry in Context** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

2.1: Atomic Theory

Learning Objectives

- Explain how all matter is composed of atoms.
- Describe the modern atomic theory.
- Recognize which elements exist as diatomic molecules.

Take some aluminum foil. Cut it in half. Now you have two smaller pieces of aluminum foil. Cut one of the pieces in half again. Cut one of those smaller pieces in half again. Continue cutting, making smaller and smaller pieces of aluminum foil.

It should be obvious that the pieces are still aluminum foil; they are just becoming smaller and smaller. But how far can you take this exercise, at least in theory? Can you continue cutting the aluminum foil into halves forever, making smaller and smaller pieces? Or is there some limit, some absolute smallest piece of aluminum foil? (Thought experiments like this—and the conclusions based on them—were debated as far back as the fifth century BC.)

The modern atomic theory, proposed about 1803 by the English chemist John Dalton (Figure **2.1.1**), is a fundamental concept that states that all elements are composed of atoms. Previously, we defined an atom as the smallest part of an element that maintains the identity of that element. Individual atoms are extremely small; even the largest atom has an approximate diameter of only 5.4×10^{-10} m. With that size, it takes over 18 million of these atoms, lined up side by side, to equal the width of your little finger (about 1 cm).

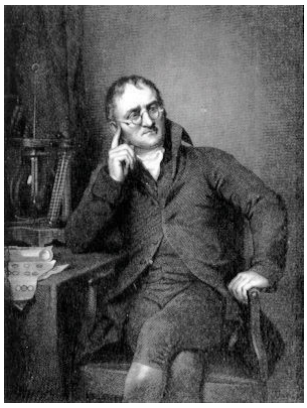


Figure **2.1.1** John Dalton was an English scientist who articulated the modern atomic theory.

Most elements in their pure form exist as **individual atoms**. For example, a macroscopic chunk of iron (Fe) metal is composed, microscopically, of individual atoms. Some elements, however, exist as groups of atoms called molecules. Several important elements exist as two-atom combinations and are called **diatomic molecules**. In representing a diatomic molecule, we use the symbol of the element and include the ***subscript*** "2" to indicate that two atoms of that element are joined together. The elements that exist as diatomic molecules are hydrogen (H_2), nitrogen (N_2), fluorine (F_2), oxygen (O_2), iodine (I_2), chlorine (Cl_2) and bromine (Br_2). A few other elements can exist as 3-atom molecules like ozone (O_3) and 4-atom molecules like phosphorus (P_4). The most common form of the element sulfur is composed of molecules that consist of eight atoms of sulfur; its molecular formula is S_8 (Figure **2.1.2**).

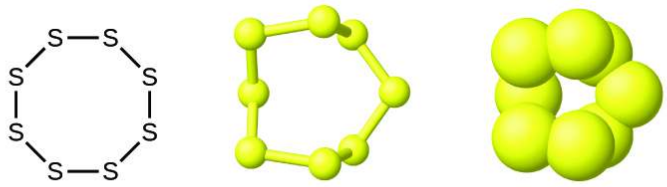


Figure **2.1.2**: A molecule of sulfur is composed of eight sulfur atoms and is therefore written as S_8. It can be represented as (a) a structural formula, (b) a ball-and-stick model, and (c) a space-filling model. Sulfur atoms are represented by yellow spheres.

Figure A shows eight sulfur atoms, symbolized with the letter S, that are bonded to each other to form an octagon. Figure B shows a 3-D, ball-and-stick model of the arrangement of the sulfur atoms. The shape is clearly not octagonal as it is represented in the structural formula. Figure C is a space-filling model that shows each sulfur atom is partially embedded into the sulfur atom it bonds with.

It is important to note that a subscript following a symbol and a number in front of a symbol do not represent the same thing; for example, H_2 and 2H represent distinctly different species. H_2 is a molecular formula; it represents a diatomic molecule of hydrogen, consisting of two atoms of the element that are chemically bonded together. The expression 2H, on the other hand, indicates two separate hydrogen atoms that are **not** combined as a unit. The expression $2H_2$ represents two molecules of diatomic hydrogen (Figure **2.1.3**).

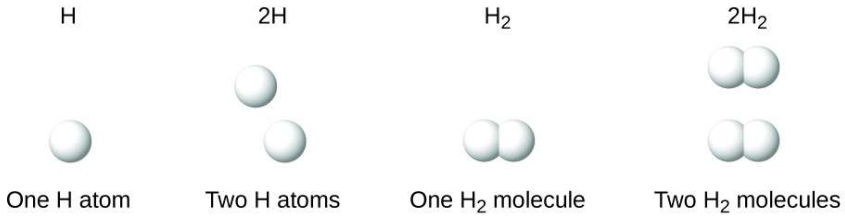


Figure **2.1.3**: The symbols H, 2H, H_2, and $2H_2$ represent very different entities.

This figure shows four diagrams. The diagram for H shows a single, white sphere and is labeled one H atom. The diagram for 2 H shows two white spheres that are not bonded together. It is labeled 2 H atoms. The diagram for H subscript 2 shows two white spheres bonded together. It is labeled one H subscript 2 molecule. The diagram for 2 H subscript 2 shows two sets of bonded, white spheres. It is labeled 2 H subscript 2 molecules.

✔ Example 2.1.1

Write the chemical formula of the following elements:

a. oxygen
b. carbon
c. potassium

Solution

Memorizing the diatomic molecules is worthwhile for our future endeavors. A mnemonic device to help in the memorization of the diatomic elements is as follows: **H**ave **N**o **F**ear **O**f **I**ce **C**old **B**eer. (hydrogen, nitrogen, fluorine, oxygen, iodine, chlorine and bromine).

a. Oxygen is one of the seven diatomic molecular elements. Its chemical formula is O_2.
b. Carbon is monatomic, hence its formula is C.
c. Potassium is monatomic hence its formula is K.

2.1.1 Exercise

Write the chemical formula of the following elements:

a. hydrogen
b. nitrogen
c. neon

Answer a

Hydrogen is one of the seven diatomic molecular elements. Its chemical formula is H_2.

Answer b

Nitrogen is one of the seven diatomic molecular elements. Its chemical formula is N_2.

Answer c

Neon is a monatomic element, hence its formula is Ne.

Looking Closer: Atomic Theory

Dalton's ideas are called the *modern* atomic theory because the concept of atoms is very old. The Greek philosophers Leucippus and Democritus originally introduced atomic concepts in the fifth century BC. (The word *atom* comes from the Greek word *atomos*, which means "indivisible" or "uncuttable.") Dalton had something that the ancient Greek philosophers didn't have, however; he had experimental evidence, such as the formulas of simple chemicals and the behavior of gases. In the 150 years or so before Dalton, natural philosophy had been maturing into modern science, and the scientific method was being used to study nature. So when Dalton announced a modern atomic theory, he was proposing a fundamental theory to describe many previous observations of the natural world; he was not just participating in a philosophical discussion.

Concept Review Exercises

1. What is the modern atomic theory?
2. What are atoms?

Answers

1. The modern atomic theory states that all matter is composed of atoms.
2. Atoms are the smallest parts of an element that maintain the identity of that element.

Key Takeaways

- **Atoms** are the ultimate building blocks of all matter.
- The modern atomic theory establishes the concepts of **atoms** and how they compose matter.
- The **diatomic** elements are hydrogen, nitrogen, fluorine, oxygen, iodine, chlorine and bromine.

2.2: Atomic Theory

2.1: Atomic Theory is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

- **2.2: Atomic Theory** by Anonymous is licensed CC BY-NC-SA 3.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

2.2: Atomic Structure

Learning Objectives

- Describe the three main subatomic particles.
- State how the subatomic particles are arranged in atoms.

There have been several minor but important modifications to Dalton's atomic theory. For one thing, Dalton considered atoms to be indivisible. We know now that atoms not only can be divided but also are composed of three different kinds of particle, *subatomic particles*, with their own properties that are different from the chemical properties of atoms.

Subatomic Particles

The first subatomic particle was identified in 1897 and called the electron. It is an extremely tiny particle, with a mass of about 9.109×10^{-31} kg. Experiments with magnetic fields showed that the electron has a negative electrical charge. By 1920, experimental evidence indicated the existence of a second particle. A proton has the same amount of charge as an electron, but its charge is positive, not negative. Another major difference between a proton and an electron is mass. Although still incredibly small, the mass of a proton is 1.673×10^{-27} kg, which is almost 2,000 times greater than the mass of an electron. Because opposite charges attract each other (while like charges repel each other), protons attract electrons (and vice versa).

Finally, additional experiments pointed to the existence of a third particle. Evidence produced in 1932 established the existence of the neutron, a particle with about the same mass as a proton but with no electrical charge, it is *neutral*. We understand now that all atoms can be broken down into subatomic particles: protons, neutrons, and electrons. Table **2.2.1** lists some of their important characteristics and the symbols used to represent each particle.

Table **2.2.1**: Properties of the Subatomic Particles

Particle	Symbol	Mass (kg)	Relative Mass (proton = 1)	Relative Charge
proton	p^+	1.673×10^{-27}	1	+1
neutron	n^0	1.675×10^{-27}	1	0
electron	e^-	9.109×10^{-31}	0.00055	−1

The Nucleus

How are these subatomic particles arranged? Between 1909 and 1911, Ernest Rutherford, a Cambridge physicist, and his associates Hans Geiger and Ernest Marsden performed experiments that provided strong evidence concerning the internal structure of an atom. They took a very thin metal foil, such as gold or platinum, and aimed a beam of positively charged particles (called alpha particles, which are combinations of two protons and two neutrons) from a radioactive source toward the foil. Surrounding the foil was a detector—either a scintillator (a material that glows when hit by such particles) or some unexposed film (which is exposed where the particles hit it). The detector allowed the scientists to determine the distribution of the alpha particles after they interacted with the foil. Figure **2.2.1** shows a diagram of the experimental setup.

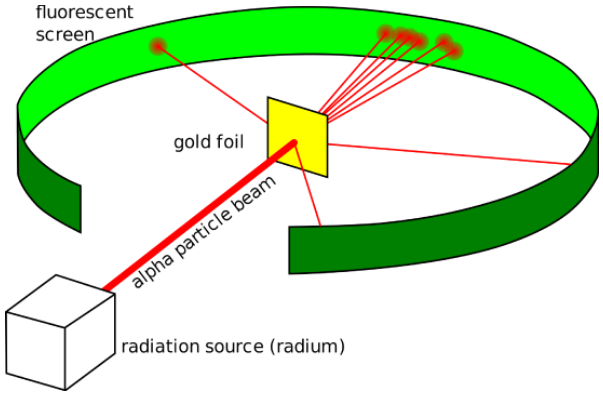


Figure **2.2.1**: The Geiger-Marsden Experimental Setup. Experiments using this setup were used to investigate the structure of atoms. In this experiment, most of the particles traveled straight through the foil, but some alpha particles were deflected off to one side. Some were even deflected back toward the source. This was unexpected. Rutherford once said, "It was almost as incredible as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you." (CC SA-BY 3.0; Kurzon).

Rutherford proposed the following model to explain these experimental results. Protons and neutrons are concentrated in a central region he called the nucleus (plural, *nuclei*) of the atom. Electrons are outside the nucleus and orbit about it because they are attracted to the positive charge in the nucleus. Most of the mass of an atom is in the nucleus, while the orbiting electrons account for an atom's size. As a result, an atom consists largely of empty space. Rutherford called his description the "planetary model" of the atom. Figure **2.2.2** shows how this model explains the experimental results.

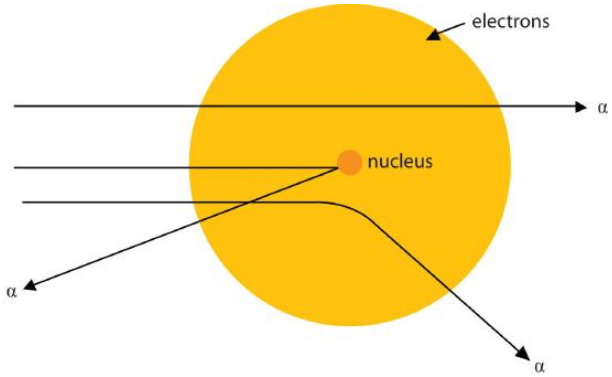


Figure **2.2.2**: Rutherford's Metal Foil Experiments. Rutherford explained the results of the metal foil experiments by proposing that most of the mass and the positive charge of an atom are located in its nucleus, while the relatively low-mass electrons orbit about the nucleus. Most alpha particles go straight through the empty space, a few particles are deflected, and fewer still ricochet back toward the source. The nucleus is much smaller proportionately than depicted here.

> *The planetary model of the atom replaced the plum pudding model, which had electrons floating around aimlessly like plums in a "pudding" of positive charge.*

Rutherford's model is essentially the same model that we use today to describe atoms but with one important modification. The planetary model suggests that electrons occupy certain specific, circular orbits about the nucleus. We know now that this model is overly simplistic. A better description is that electrons form fuzzy clouds around nuclei. Figure **2.2.3** shows a more modern version of our understanding of atomic structure.

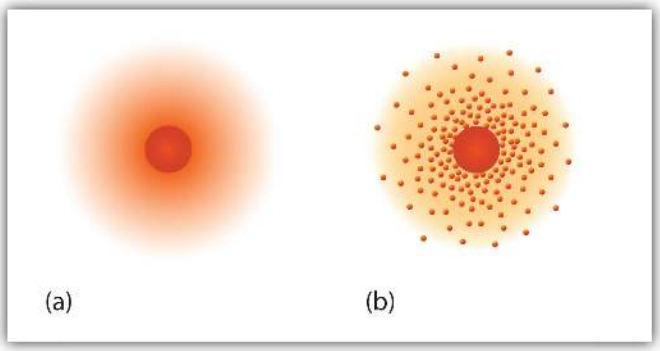


Figure **2.2.3**: A Modern Depiction of Atomic Structure. A more modern understanding of atoms, reflected in these representations of the electron in a hydrogen atom, is that electrons occupy regions of space about the nucleus; they are not in discrete orbits like planets around the sun. (a) The darker the color, the higher the probability that an electron will be at that point. (b) In a two-dimensional cross section of the electron in a hydrogen atom, the more crowded the dots, the higher the probability that an electron will be at that point. In both (a) and (b), the nucleus is in the center of the diagram.

Concept Review Exercises

1. What are the charges and the relative masses of the three subatomic particles?
2. Describe the structure of an atom in terms of its protons, neutrons, and electrons.

Answers

1. proton: +1, large; neutron: 0, large; electron: −1, small
2. Protons and neutrons are located in a central nucleus, while electrons orbit about the nucleus.

Key Takeaways

- Atoms are composed of three main subatomic particles: protons, neutrons, and electrons.
- Protons and neutrons are grouped together in the nucleus of an atom, while electrons orbit about the nucleus.

This page titled 2.2: Atomic Structure is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous via source content that was edited to the style and standards of the LibreTexts platform.

- **2.3: The Structure of Atoms** by Anonymous is licensed CC BY-NC-SA 3.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

2.2.1: Nuclei of Atoms

Learning Objectives

- Define and differentiate between the atomic number and the mass number of an element.
- Explain how isotopes differ from one another.

Now that we know how atoms are generally constructed, what do atoms of any particular element look like? How many protons, neutrons, and electrons are in a specific kind of atom? First, if an atom is electrically neutral overall, then the number of protons equals the number of electrons. Because these particles have the same but opposite charges, equal numbers cancel out, producing a neutral atom.

Atomic Number

In the 1910s, experiments with x-rays led to this useful conclusion: the magnitude of the positive charge in the nucleus of every atom of a particular element is the same. In other words, all atoms of the same element have the same number of protons. Furthermore, different elements have a different number of protons in their nuclei, so the number of protons in the nucleus of an atom is characteristic of a particular element. This discovery was so important to our understanding of atoms that the number of protons in the nucleus of an atom is called the atomic number (Z).

For example, hydrogen has the atomic number 1; all hydrogen atoms have 1 proton in their nuclei. Helium has the atomic number 2; all helium atoms have 2 protons in their nuclei. There is no such thing as a hydrogen atom with 2 protons in its nucleus; a nucleus with 2 protons would be a helium atom. The atomic number *defines* an element. Table **2.2.1.1** lists some common elements and their atomic numbers. Based on its **atomic number**, you can determine the **number of protons in the nucleus** of an atom. The largest atoms have over 100 protons in their nuclei.

Example 2.2.1.1

What is the number of protons in the nucleus of each element?

a. aluminum
b. iron
c. carbon

Answer a

According to Table 2.4.1, aluminum has an atomic number of 13. Therefore, every aluminum atom has 13 protons in its nucleus.

Answer b

Iron has an atomic number of 26. Therefore, every iron atom has 26 protons in its nucleus.

Answer c

Carbon has an atomic number of 6. Therefore, every carbon atom has 6 protons in its nucleus.

Exercise 2.2.1.1

What is the number of protons in the nucleus of each element? Use Table 2.4.1.

a. sodium
b. oxygen
c. chlorine

Answer a

Sodium has 11 protons in its nucleus.

Answer b

Oxygen has 8 protons in its nucleus.

Answer c

Chlorine has 17 protons in its nucleus

How many electrons are in an atom? Previously we said that for an electrically neutral atom, the **number of electrons equals the number of protons**, so the total opposite charges cancel. Thus, the **atomic number** of an element also gives the **number of electrons** in an atom of that element. (Later we will find that some elements may gain or lose electrons from their atoms, so those atoms will no longer be electrically neutral. Thus we will need a way to differentiate the number of electrons for those elements.)

Example 2.2.1.2

How many electrons are present in the atoms of each element?

a. sulfur
b. tungsten
c. argon

Answer a

The atomic number of sulfur is 16. Therefore, in a neutral atom of sulfur, there are 16 electrons.

Answer b

The atomic number of tungsten is 74. Therefore, in a neutral atom of tungsten, there are 74 electrons.

Answer c

The atomic number of argon is 18. Therefore, in a neutral atom of argon, there are 18 electrons.

Exercise 2.2.1.2

How many electrons are present in the atoms of each element?

a. magnesium
b. potassium
c. iodine

Answer a

Mg has 12 electrons.

Answer b

K has 19 electrons.

Answer c

I has 53 electrons.

Table **2.2.1.1**: Some Common Elements and Their Atomic Numbers

Element	Atomic Number	Element	Atomic Nmbers
aluminum (Al)	13	magnesium (Mg)	12
americium (Am)	95	manganese (Mn)	25
argon (Ar)	18	mercury (Hg)	80
barium (Ba)	56	neon (Ne)	10
beryllium (Be)	4	nickel (Ni)	28
bromine (Br)	35	nitrogen (N)	7
calcium (Ca)	20	oxygen (O)	8
carbon (C)	6	phosphorus (P)	15
chlorine (Cl)	17	platinum (Pt)	78
chromium (Cr)	24	potassium (K)	19
cesium (Cs)	55	radon (Rn)	86
fluorine (F)	9	silver (Ag)	47
gallium (Ga)	31	sodium (Na)	11
gold (Au)	79	strontium (Sr)	38
helium (He)	2	sulfur (S)	16
hydrogen (H)	1	titanium (Ti)	22
iron (Fe)	26	tungsten (W)	74
iodine (I)	53	uranium (U)	92
lead (Pb)	82	zinc (Zn)	30
lithium (Li)	3	zirconium (Zr)	40

Isotopes

How many neutrons are in atoms of a particular element? At first it was thought that the number of neutrons in a nucleus was also characteristic of an element. However, it was found that atoms of the same element can have *different* numbers of neutrons. Atoms of the same element (i.e., same atomic number, Z) that have different numbers of neutrons are called isotopes. For example, 99% of the carbon atoms on Earth have 6 neutrons and 6 protons in their nuclei; about 1% of the carbon atoms have 7 neutrons in their nuclei. Naturally occurring carbon on Earth, therefore, is actually a mixture of isotopes, albeit a mixture that is 99% carbon with 6 neutrons in each nucleus.

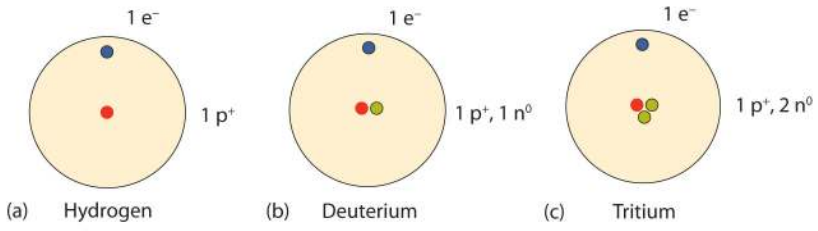


Figure **2.2.1.1**: Isotopes of Hydrogen. Most hydrogen atoms have only a proton in the nucleus (a). A small amount of hydrogen exists as the isotope deuterium, which has one proton and one neutron in its nucleus (b). A tiny amount of the hydrogen isotope tritium, with one proton and two neutrons in its nucleus, also exists on Earth (c). The nuclei and electrons are proportionately much smaller than depicted here.

An important series of isotopes is found with hydrogen atoms. Most hydrogen atoms have a nucleus with only a single proton. About 1 in 10,000 hydrogen nuclei, however, also has a neutron; this particular isotope is called *deuterium*. An extremely rare hydrogen isotope, *tritium*, has 1 proton and 2 neutrons in its nucleus. Figure **2.2.1.1** compares the three isotopes of hydrogen.

> The discovery of isotopes required a minor change in Dalton's atomic theory. Dalton thought that all atoms of the same element were exactly the same.

Most elements exist as mixtures of isotopes. In fact, there are currently over 3,500 isotopes known for all the elements. When scientists discuss individual isotopes, they need an efficient way to specify the number of neutrons in any particular nucleus. The *mass number* (A) of an atom is the sum of the numbers of protons and neutrons in the nucleus. Given the mass number for a nucleus (and knowing the atomic number of that particular atom), you can determine the number of neutrons by subtracting the atomic number from the mass number.

A simple way of indicating the mass number of a particular isotope is to list it as a superscript on the left side of an element's symbol. Atomic numbers are often listed as a subscript on the left side of an element's symbol. Thus, we might see

$$\begin{matrix}\text{mass number}\longrightarrow 56\\ \text{atomic number}\longrightarrow 26\end{matrix}\mathrm{Fe} \tag{2.2.1.1}$$

which indicates a particular isotope of iron. The 26 is the atomic number (which is the same for all iron atoms), while the 56 is the mass number of the isotope. To determine the number of neutrons in this isotope, we subtract 26 from 56: 56 − 26 = 30, so there are 30 neutrons in this atom.

✔ Example 2.2.1.3

How many protons and neutrons are in each atom?

a. $^{35}_{17}\mathrm{Cl}$
b. $^{127}_{53}\mathrm{I}$

Answer a

In $^{35}_{17}\mathrm{Cl}$ there are 17 protons, and 35 − 17 = 18 neutrons in each nucleus.

Answer b

In $^{127}_{53}\mathrm{I}$ there are 53 protons, and 127 − 53 = 74 neutrons in each nucleus.

? Exercise 2.2.1.3

How many protons and neutrons are in each atom?

a. $^{197}_{79}\mathrm{Au}$
b. $^{23}_{11}\mathrm{Na}$

Answer a

In $^{197}_{79}\mathrm{Au}$ there are 79 protons, and 197 − 79 = 118 neutrons in each nucleus.

Answer b

In $^{23}_{11}\mathrm{Na}$ there are 11 protons, and 23 − 11 = 12 neutrons in each nucleus.

It is not absolutely necessary to indicate the atomic number as a subscript because each element has its own unique atomic number. Many isotopes are indicated with a superscript only, such as $^{13}\mathrm{C}$ or $^{235}\mathrm{U}$. You may also see isotopes represented in print as, for example, carbon-13 or uranium-235.

Summary

The atom consists of discrete particles that govern its chemical and physical behavior. Each atom of an element contains the same number of protons, which is the **atomic number (Z)**. Neutral atoms have the same number of electrons and protons. Atoms of an element that contain different numbers of neutrons are called **isotopes**. Each isotope of a given element has the same atomic number but a different **mass number (A)**, which is the **sum of the numbers of protons and neutrons**.

Almost all of the mass of an atom is from the total protons and neutrons contained within a tiny (and therefore very dense) nucleus. The majority of the volume of an atom is the surrounding space in which the electrons reside. A representation of a carbon-12 atom is shown below in Figure **2.2.1.2**.

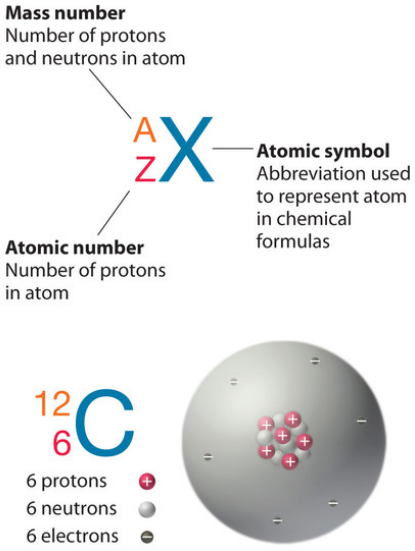


Figure **2.2.1.2**: Formalism used for identifying specific nuclide (any particular kind of nucleus)

The atomic symbol, X, is the abbreviation used to represent an atom in chemical formulas. The mass number, A, is the number of protons and neutrons in the atom, which is to the left of the X. The atomic number, Z, is the number of protons in the atom, which is to the left of the X and below the A.

Concept Review Exercises

1. Why is the atomic number so important to the identity of an atom?
2. What is the relationship between the number of protons and the number of electrons in an atom?
3. How do isotopes of an element differ from each other?
4. What is the mass number of an element?

Answers

1. The atomic number defines the identity of an element. It describes the number of protons in the nucleus.
2. In an electrically neutral atom, the number of protons equals the number of electrons.
3. Isotopes of an element have the same number of protons but have different numbers of neutrons in their nuclei.
4. The mass number is the sum of the numbers of protons and neutrons in the nucleus of an atom.

Key Takeaways

- Each element is identified by its atomic number. The atomic number provides the element's location on the periodic table
- The isotopes of an element have different masses and are identified by their mass numbers.

This page titled 2.2.1: Nuclei of Atoms is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous via source content that was edited to the style and standards of the LibreTexts platform.

- **2.4: Nuclei of Atoms** by Anonymous is licensed CC BY-NC-SA 3.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

2.3: Atomic Masses

Learning Objectives

- Define atomic mass and atomic mass unit.
- Calculate atomic mass.

Even though atoms are very tiny pieces of matter, they have mass. Their masses are so small, however, that chemists often use a unit other than grams to express them—the atomic mass unit.

Atomic Mass Unit

The atomic mass unit (abbreviated u, although amu is also used) is defined as 1/12 of the mass of a ^{12}C atom:

$$1\ \text{u} = \frac{1}{12}\ \text{the mass of}\ ^{12}\text{C atom} \tag{2.3.1}$$

It is equal to 1.661×10^{-24} g.

Masses of other atoms are expressed with respect to the atomic mass unit. For example, the mass of an atom of ^{1}H is 1.008 u, the mass of an atom of ^{16}O is 15.995 u, and the mass of an atom of ^{32}S is 31.97 u. Note, however, that these masses are for particular isotopes of each element. Because most elements exist in nature as a mixture of isotopes, any sample of an element will actually be a mixture of atoms having slightly different masses (because neutrons have a significant effect on an atom's mass). How, then, do we describe the mass of a given element? By calculating an average of an element's atomic masses, weighted by the natural abundance of each isotope, we obtain a weighted average mass called the atomic mass (also commonly referred to as the *atomic weight*) of an element.

Atomic Mass is the Weighted Average Mass of Isotopes

As stated above, most elements occur naturally as a mixture of two or more isotopes. Listed below (Table **2.3.1**) are the naturally occurring isotopes of selected elements along with the percent natural abundance of each.

Table **2.3.1**: Atomic Masses and Percent Abundances of Some Natural Isotopes

Element	Isotope (Symbol)	Percent Natural Abundance	Atomic Mass (amu)	Average Atomic Mass (amu)
Hydrogen	$^{1}_{1}H$	99.985	1.0078	1.0079
	$^{2}_{1}H$	0.015	2.0141	
	$^{3}_{1}H$	negligible	3.0160	
Carbon	$^{12}_{6}C$	98.89	12.000	12.011
	$^{13}_{6}C$	1.11	13.003	
	$^{14}_{6}C$	trace	14.003	
Oxygen	$^{16}_{8}O$	99.759	15.995	15.999
	$^{17}_{8}O$	0.037	16.995	
	$^{18}_{8}O$	0.204	17.999	
Chlorine	$^{35}_{17}Cl$	75.77	34.969	35.453
	$^{38}_{17}Cl$	24.23	36.966	
Copper	$^{63}_{29}Cu$	69.17	62.930	63.546
	$^{65}_{29}Cu$	30.83	64.928	

For some elements, one particular isotope is much more abundant than any other isotopes. For example, naturally occurring hydrogen is nearly all hydrogen-1, and naturally occurring oxygen is nearly all oxygen-16. For many other elements, however, more than one isotope may exist in substantial quantities. Chlorine (atomic number 17) is yellowish-green toxic gas. About three quarters of all chlorine atoms have 18 neutrons, giving those atoms a mass number of 35. About one quarter of all chlorine atoms have 20 neutrons, giving those atoms a mass number of 37. Were you to simply calculate the arithmetic average of the precise atomic masses, you would get approximately 36.

$$\frac{34.969\,u + 36.966\,u}{2} = 35.968\,u$$

As you can see, the average atomic mass given in the last column of the table above (35.453) is significantly lower. Why? The reason is that we need to take into account the natural abundance percentages of each isotope in order to calculate what is called the **weighted average**. The atomic mass *of an element is the weighted average of the atomic masses of the naturally occurring isotopes of that element.*

$$0.7577\,(34.969\,u) + 0.2423\,(36.966\,u) = 35.453\,u$$

The weighted average is determined by multiplying the percent of natural abundance by the actual mass of the isotope. This is repeated until there is a term for each isotope. For chlorine, there are only two naturally occurring isotopes so there are only two terms.

Atomic mass = (%1)(mass 1) + (%2)(mass 2) + ⋯

Another example: oxygen exists as a mixture that is 99.759% ^{16}O, 0.037% ^{17}O and 0.204% ^{18}O. The atomic mass of oxygen (use percent natural abundance data from Table 2.5.1) would be calculated as follows:

Atomic mass = (%1)(mass 1) + (%2)(mass 2) + (%3)(mass 3)

$$0.99759\,(15.995u) + 0.00037\,(16.995u) + 0.00204\,(17.999u) = 15.999u$$

To confirm your answer, compare the calculated value to the weighted mass displayed on the periodic table.

Example 2.3.1

Calculate the atomic mass of oxygen. Oxygen exists as a mixture of 3 isotopes. Their respective masses and natural abundance are shown below.

- ^{16}O: 15.995 u (99.759%)
- ^{17}O: 16.995 u (0.037%)
- ^{18}O: 17.999 u (0.204%)

Solution

Multiply the isotope abundance by the actual mass of the isotope, and then sum up the products.

$$0.99759\,(15.995\,u) + 0.00037\,(16.995\,u) + 0.00204\,(17.999\,u) = 15.999\,u$$

2.3.1 Exercise

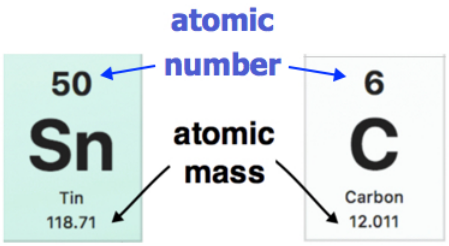
Calculate the atomic mass of copper. Copper exists as a mixture of 2 isotopes. Their respective masses and natural abundance are shown below.

- ^{63}Cu: 62.930 u (69.17%)
- ^{65}Cu: 64.928 u (30.83%)

Answer

63.546 u

The **atomic mass** of each element is found under the element symbol in the **periodic table.** Examples are shown below. The atomic mass of tin (Sn) is 118.71 u while the atomic mass of carbon (C) is 12.011 u. On the other hand, the **atomic number (Z)** of each element is found **above** the atomic symbol.



Atomic mass indicated on entries of the Periodic Table. (public Domain; Pubchem)

The **periodic table** is found in this link:

https://pubchem.ncbi.nlm.nih.gov/periodic-table/png/Periodic_Table_of_Elements_w_Atomic_Mass_PubChem.png

Example 2.3.2: Mass of Carbon

What is the average mass of a carbon atom in grams? The atomic mass is found in the Periodic Table. Please use two decimal places.

Solution

This is a simple one-step conversion, similar to conversions we did in Chapter 1. We use the fact that 1 u = 1.661×10^{-24} g:

$$12.01\ \cancel{u} \times \frac{1.661 \times 10^{-24}\ \text{g}}{1\ \cancel{u}} = 1.995 \times 10^{-23}\ \text{g}$$

This is an extremely small mass, which illustrates just how small individual atoms are.

? Exercise 2.3.2: Mass of Tin

What is the average mass of a tin atom in grams? The average atomic mass is found in the Periodic Table. Please use two decimal places.

Answer

$$118.71 \cancel{u} \times \frac{1.661 \times 10^{-24}\ \text{g}}{1\ \cancel{u}} = 1.972 \times 10^{-22}\ \text{g}$$

Concept Review Exercises

1. Define atomic mass. Why is it considered a weighted average?
2. What is an atomic mass unit?

Answers

1. The atomic mass is an average of an element's atomic masses, weighted by the natural abundance of each isotope of that element. It is a weighted average because different isotopes have different masses.
2. An atomic mass unit is 1/12th of the mass of a ^{12}C atom.

Key Takeaway

- Atoms have a mass that is based largely on the number of protons and neutrons in their nucleus.
- The atomic mass of each element in the Periodic Table is the weighted average of the mass of all its isotopes.

This page titled 2.3: Atomic Masses is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous via source content that was edited to the style and standards of the LibreTexts platform.

- **2.5: Atomic Masses** by Anonymous is licensed CC BY-NC-SA 3.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

2.4: Electronic Structure in Atoms

Learning Objectives

- Describe how electrons are grouped within atoms.

Although we have discussed the general arrangement of subatomic particles in atoms, we have said little about how electrons occupy the space about the nucleus. Do they move around the nucleus at random, or do they exist in some ordered arrangement?

The modern theory of electron behavior is called quantum mechanics. It makes the following statements about electrons in atoms:

- Electrons in atoms can have only certain specific energies. We say that the energies of the electrons are quantized.
- Electrons are organized according to their energies into sets called **shells** (labeled by the principle quantum number, ***n***). Generally the higher the energy of a shell, the farther it is (on average) from the nucleus. Shells do not have specific, fixed distances from the nucleus, but an electron in a higher-energy shell will spend more time farther from the nucleus than does an electron in a lower-energy shell.
- Shells are further divided into subsets of electrons called **subshells**. The first shell has only one subshell, the second shell has two subshells, the third shell has three subshells, and so on. The subshells of each shell are labeled, in order, with the letters *s*, *p*, *d*, and *f*. Thus, the first shell has only a single *s* subshell (called **1*s***), the second shell has **2*s*** and **2*p*** subshells, the third shell has **3*s***, **3*p***, and **3*d*** and so forth.

Table **2.4.1**: Shells and Subshells

Shell	Number of Subshells	Names of Subshells
1	1	*1s*
2	2	*2s* and *2p*
3	3	*3s*, *3p* and *3d*
4	4	*4s*, *4p*, *4d* and *4f*

- Different subshells hold a different maximum number of electrons. **Any *s* subshell can hold up to 2 electrons; *p*, 6; *d*, 10; and *f*, 14.**

Table **2.4.2**: Number of Electrons

Subshell	Maximum Number of Electrons
s	2
p	6
d	10
f	14

It is the arrangement of electrons into shells and subshells that most concerns us here, so we will focus on that.

We use numbers to indicate which shell an electron is in. As shown in Table **2.4.1**, the first shell, closest to the nucleus and with the lowest-energy electrons, is shell 1. This first shell has only one subshell, which is labeled 1*s* and can hold a maximum of 2 electrons. We combine the shell and subshell labels when referring to the organization of electrons about a nucleus and use a superscript to indicate how many electrons are in a subshell. Thus, because a hydrogen atom has its single electron in the *s* subshell of the first shell, we use $\mathbf{1}s^{\mathbf{1}}$ to describe the electronic structure of hydrogen. This structure is called an electron configuration. Electron configurations are shorthand descriptions of the arrangements of electrons in atoms. The electron configuration of a hydrogen atom is spoken out loud as “one-ess-one.”

Helium atoms have 2 electrons. Both electrons fit into the 1*s* subshell because *s* subshells can hold up to 2 electrons; therefore, the electron configuration for helium atoms is $\mathbf{1}s^2$ (spoken as “one-ess-two”).

The 1*s* subshell cannot hold 3 electrons (because an *s* subshell can hold a maximum of 2 electrons), so the electron configuration for a lithium atom cannot be $1s^3$. Two of the lithium electrons can fit into the 1*s* subshell, but the third electron must go into the second shell. The second shell has two subshells, *s* and *p*, which fill with electrons in that order. The 2*s* subshell holds a maximum of 2 electrons, and the 2*p* subshell holds a maximum of 6 electrons. Because lithium’s final electron goes into the 2*s* subshell, we write the electron configuration of a lithium atom as $\mathbf{1}s^2\mathbf{2}s^1$**.** The shell diagram for a lithium atom is shown below. The shell closest to the nucleus (first shell) has 2 dots representing the 2 electrons in **1*s***, while the outermost shell (**2*s***) has 1 electron.

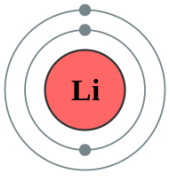


Figure **2.4.1**: Shell diagram of lithium (Li) atom.

The next largest atom, beryllium, has 4 electrons, so its electron configuration is $1s^22s^2$. Now that the 2*s* subshell is filled, electrons in larger atoms start filling the 2*p* subshell. Thus, the electron configurations for the next six atoms are as follows:

- B: $1s^22s^22p^1$
- C: $1s^22s^22p^2$
- N: $1s^22s^22p^3$
- O: $1s^22s^22p^4$
- F: $1s^22s^22p^5$
- Ne: $1s^22s^22p^6$

With neon, the 2*p* subshell is completely filled. Because the second shell has only two subshells, atoms with more electrons now must begin the third shell. The third shell has three subshells, labeled *s*, *p*, and *d*. The *d* subshell can hold a maximum of 10 electrons. The first two subshells of the third shell are filled in order—for example, the electron configuration of aluminum, with 13 electrons, is $1s^22s^22p^63s^23p^1$. However, a curious thing happens after the 3*p* subshell is filled: the 4*s* subshell begins to fill before the 3*d* subshell does. In fact, the exact ordering of subshells becomes more complicated at this point (after argon, with its 18 electrons), so we will not consider the electron configurations of larger atoms. A fourth subshell, the *f* subshell, is needed to complete the electron configurations for all elements. An *f* subshell can hold up to 14 electrons.

Electron filling always starts with **1*s***, the subshell closest to the nucleus. Next is **2*s*, 2*p*, 3*s*, 3*p*, 4*s*, 3*d*, 4*p*, 5s, 4d, 5p, 6s,** etc., shown in the electron shell filling order diagram in Figure **2.4.2**. Follow each arrow in order **from top to bottom**. The subshells you reach along each arrow give the ordering of filling of subshells in larger atoms.

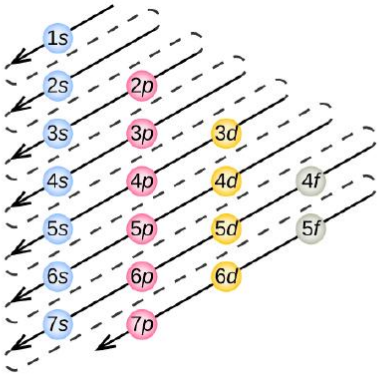


Figure **2.4.2**: The order of electron filling in an atom.

Example 2.4.1: Electronic Configuration of Phosphorus Atoms

Using Figure **2.4.2** as your guide, write the electron configuration of a neutral phosphorus atom. The atomic number of P is 15.

Solution

A neutral phosphorus atom has 15 electrons. Two electrons can go into the 1*s* subshell, 2 can go into the 2*s* subshell, and 6 can go into the 2*p* subshell. That leaves 5 electrons. Of those 5 electrons, 2 can go into the 3*s* subshell, and the remaining 3 electrons can go into the 3*p* subshell. Thus, the electron configuration of neutral phosphorus atoms is $1s^2 2s^2 2p^6 3s^2 3p^3$.

? Exercise 2.4.1: Electronic Configuration of Chlorine Atoms

Using Figure **2.4.2** as your guide, write the electron configuration of a neutral chlorine atom. The atomic number of Cl is 17.

Answer

A neutral chlorine atom has 17 electrons. Two electrons can go into the 1*s* subshell, 2 can go into the 2*s* subshell, and 6 can go into the 2*p* subshell. That leaves 7 electrons. Of those 7 electrons, 2 can go into the 3*s* subshell, and the remaining 5 electrons can go into the 3*p* subshell. Thus, the electron configuration of neutral chlorine atoms is $1s^2 2s^2 2p^6 3s^2 3p^5$.

Since the arrangement of the periodic table is based on the electron configurations, Figure **2.4.3** provides an alternative method for determining the electron configuration. The filling order simply **begins at the top left,** with hydrogen (Z=1) and includes each subshell as you proceed in increasing atomic number (*Z*) order.

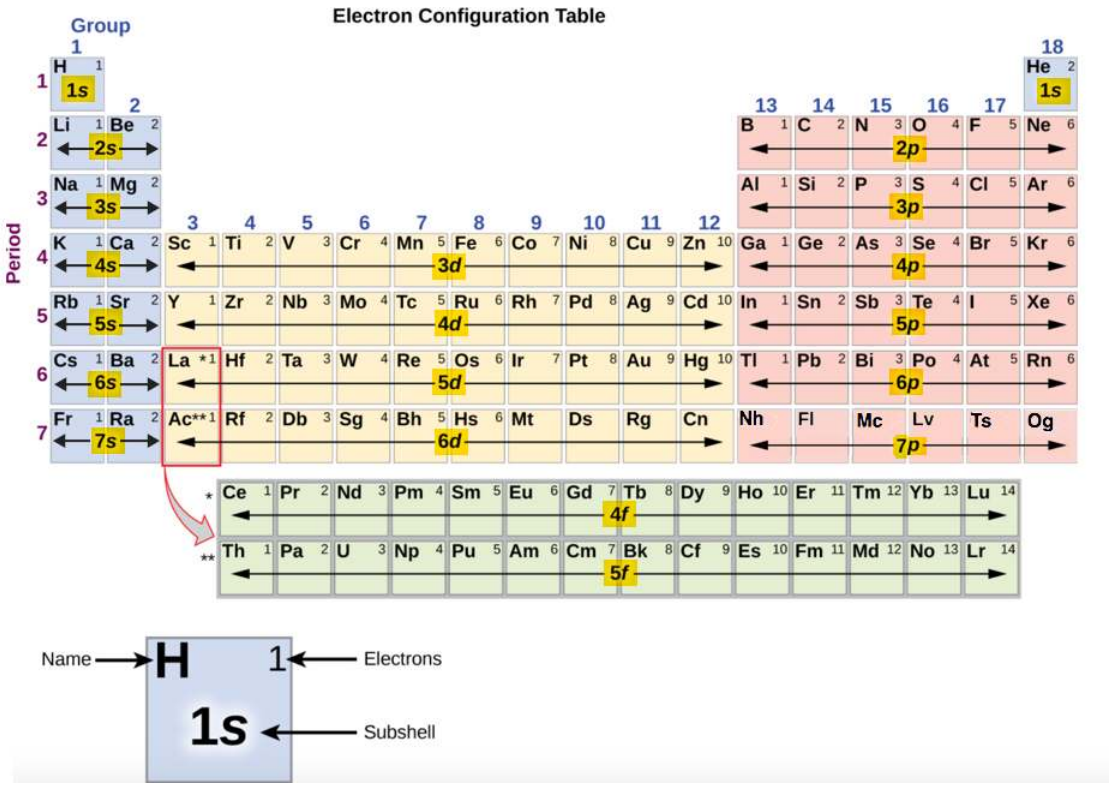


Figure **2.4.3**: This periodic table shows the electron configuration for each subshell. By "building up" from hydrogen, this table can be used to determine the electron configuration for any atom on the periodic table.

For example, the first row (Period 1) contains H and He only, because only two electrons are required to fill the 1s subshell. The second row s-block, contains only two elements, Li and Be, to fill the 2s subshell. This is followed by the second row p-block, containing 6 elements (B through Ne) since six electrons are required to fill the 2p subshell. The third row is similar to the second row elements. Two electrons are needed (Na and Mg) to fill the 3s subshell and six electrons are required (Al through Ar) to complete the 3p subshell. After filling the 3*p* block up to Ar, we see the next subshell will be 4s (K, Ca), followed by the 3*d* subshell, which are filled by ten electrons (Sc through Zn). The 4p subshell is filled next by six electrons (Ga through Kr). As you can see, the periodic table shown in Figure **2.4.3** provides a simple way to remember the order of filling the subshells in determining the electron configuration. The order of filling subshells is the same: **1s, 2*s*, 2*p*, 3*s*, 3*p*, 4*s*, 3*d*, 4*p*, 5s, 4d, 5p, 6s,** etc.

✔ Example 2.4.2: Aluminum

Using Figure **2.4.3** as your guide, write the electron configuration of neutral aluminum atom. The atomic number of Al is 13.

Solution

Aluminum has 13 electrons.

Start at Period 1 of the periodic table, Figure **2.4.3**. Place two electrons in the 1s subshell (**$1s^2$**).

Proceed to Period 2 (left to right direction). Place the next two electrons in the 2s subshell (**$2s^2$**) and the next six electrons in the 2p subshell (**$2p^6$**).

Proceed to Period 3 (left to right direction). Place the next two electrons in the 3s subshell (**$3s^2$**) and the last one electron in the 3p subshell (**$3p^1$**).

The electron configuration of Aluminum is **$1s^2 2s^2 2p^6 3s^2 3p^1$**

2.4.2 Exercise

Using Figure **2.4.3** as your guide, write the electron configuration of the atom that has 20 electrons

Answer

Start at Period 1 of Figure **2.4.3**. Place two electrons in the 1s subshell (**$1s^2$**).

Proceed to Period 2 (left to right direction). Place the next two electrons in the 2s subshell (**$2s^2$**) and the next six electrons in the 2p subshell (**$2p^6$**).

Proceed to Period 3 (left to right direction). Place the next two electrons in the 3s subshell (**$3s^2$**) and the next six electron in the 3p subshell (**$3p^6$**).

Proceed to Period 4. Place the remaining two electrons in the 4s subshell (**$4s^2$).**

The electron configuration is **$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$**

Valence Electrons

In the study of chemical reactivity, we will find that the electrons in the outermost principal energy level are very important and so they are given a special name. **Valence electrons** are the electrons in the highest occupied principal energy level of an atom.

In the second period elements, the two electrons in the **1*s*** sublevel are called **inner-shell electrons** and are not involved directly in the element's reactivity or in the formation of compounds. Lithium has a single electron in the second principal energy level and so we say that lithium has one valence electron. Beryllium has two valence electrons. How many valence electrons does boron have? You must recognize that the second principal energy level consists of both the **2*s*** and the **2*p*** sublevels and so the answer is three. In fact, the number of valence electrons goes up by one for each step across a period until the last element is reached. Neon, with its configuration ending in **$2s^2 2p^6$**, has eight valence electrons.

The alkali metal sodium (atomic number 11) has one more electron than the neon atom. This electron must go into the lowest-energy subshell available, the 3*s* orbital, giving a $1s^2 2s^2 2p^6 3s^1$ configuration. The electrons occupying the outermost shell orbital(s) (highest value of *n*) are called valence electrons, and those occupying the inner shell orbitals are called **core electrons** (Figure

\PageIndex4). Since the core electron shells correspond to noble gas electron configurations, we can abbreviate electron configurations by writing the noble gas that matches the core electron configuration, along with the valence electrons in a condensed format. For our sodium example, the symbol [Ne] represents core electrons, ($1s^2 2s^2 2p^6$) and our abbreviated or condensed configuration is [Ne]$3s^1$.

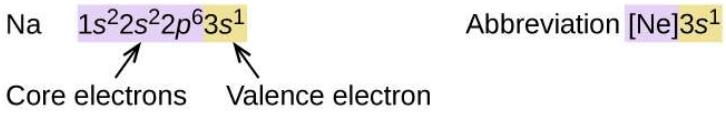


Figure **2.4.4**: A core-abbreviated electron configuration (right) replaces the core electrons with the noble gas symbol whose configuration matches the core electron configuration of the other element.

Similarly, the abbreviated configuration of lithium can be represented as [He]$2s^1$, where [He] represents the configuration of the helium atom, which is identical to that of the filled inner shell of lithium. Writing the configurations in this way emphasizes the similarity of the configurations of lithium and sodium. Both atoms, which are in the alkali metal family, have only one electron in a valence *s* subshell outside a filled set of inner shells.

Li : [He] $2s^1$
Na : [Ne] $3s^1$

A chemical reaction results from electron removal, electron addition, or electron sharing of the valence electrons of the different atoms. The path a specific element will take depends on where the electrons are in the atom and how many there are. Thus, it is convenient to separate electrons into two groups. Valence shell electrons (or, more simply, the *valence electrons*) are the electrons in the highest-numbered shell, or valence shell, while core electrons are the electrons in lower-numbered shells. We can see from the electron configuration of a carbon atom—$1s^2 2s^2 2p^2$—that it has 4 valence electrons ($2s^2 2p^2$) and 2 core electrons ($1s^2$). You will see in the next chapters that the chemical properties of elements are determined by the number of valence electrons.

Example 2.4.3

Examine the electron configuration of neutral phosphorus atoms in Example **2.4.1**, $1s^2 2s^2 2p^6 3s^2 3p^3$ and write the abbreviated notation.

Solution

Phosphorus has electron configuration, $1s^2 2s^2 2p^6 3s^2 3p^3$.

The highest-numbered shell is the third shell ($3s^2 3p^3$): **2 electrons** in the 3*s* subshell and **3 electrons** in the 3*p* subshell. That gives a total of **5 valence electrons**.

The 10 inner shell (core) electrons, $1s^2 2s^2 2p^6$ can be replaced by [Ne] (see Figure **2.4.3**). Abbreviated notation is : [Ne]$3s^2 3p^3$

Exercise 2.4.3

Examine the electron configuration of neutral calcium atom (Exercise **2.4.2**), $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$, and write the abbreviated notation.

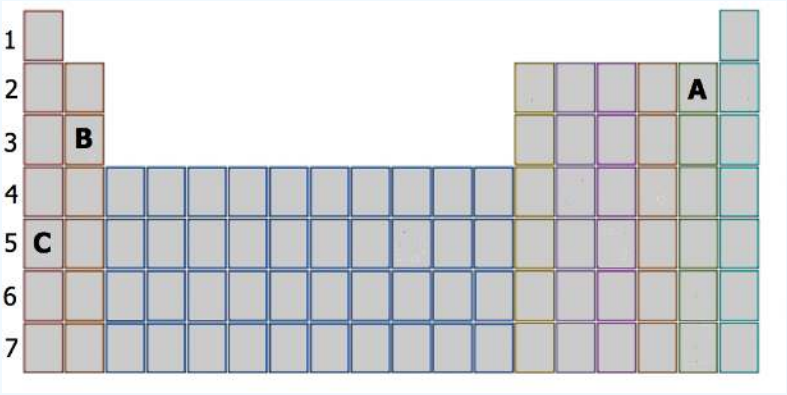
Answer

The highest-numbered shell is the fourth shell $4s^2$, which has **2 electrons** in the *4s* subshell. Hence, Calcium has **2 valence electrons**.

The 18 inner-shell (core) electrons, $1s^2 2s^2 2p^6 3s^2 3p^6$, can be replaced by [Ar], see Figure **2.4.3**. The abbreviated notation is: [Ar]$4s^2$

Example 2.4.4

Based on their respective locations in the periodic table (use Figure **2.4.3**), determine the number of valence electrons and the valence shell configuration of elements A, B and C.



Solution

Element A is located in Period 2, the *5th position* in *2p*-block. Before the electrons are placed in *2p* subshell, the *2s* subshell must be filled first. This means that A has ***two valence electrons*** in 2s (**$2s^2$**) and ***five valence electrons*** in 2p (**$2p^5$**). Answer: **$2s^2 2p^5$.** It has ***2 + 5 = 7*** **valence electrons.**

Element B is located in Period 3, the *2nd position* in *3s*-block. This means that B has ***two valence electrons*** in 3s (**$3s^2$**). Answer: **$3s^2$.**

Element C is located in Period 5, the *1st position* in *5s*-block). This means that there is only **one valence electron** in 5s (**$5s^1$**). Answer: **$5s^1$**.

2.4.4 Exercise

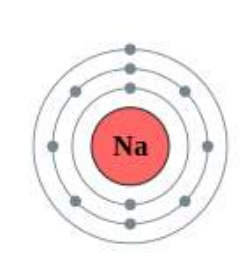
Using the location of Na is the periodic table (Figure **2.4.3**), draw the shell diagram of sodium atom.

Answer

Sodium (Na) is the first element in the 3rd row (Period 3) in the periodic table. This means that the first shell and second shells of Na atom are filled to the maximum number of electrons.

The first shell **(1s)** *is filled with* ***2 electrons***. The second shell (2s and 2p) has a **total of *8 electrons***. And, the third (last) shell has ***1 electron***.

The shell diagram of the Na atom is shown below. The shell nearest the nucleus (first shell) has 2 electrons (2 dots), the second shell has 8 electrons and the last (outermost) shell has 1 electron. (**2.8.1**)



Concept Review Exercises

1. How are electrons organized in atoms?
2. What information does an electron configuration convey?

3. What is the difference between core electrons and valence electrons?

Answers

1. Electrons are organized into shells and subshells around nuclei.
2. The electron configuration states the arrangement of electrons in shells and subshells.
3. Valence electrons are in the highest-numbered shell; all other electrons are core electrons.

Key Takeaway

- Electrons are organized into shells and subshells about the nucleus of an atom.
- The valence electrons determine the reactivity of an atom.

Exercises

This page titled 2.4: Electronic Structure in Atoms is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous via source content that was edited to the style and standards of the LibreTexts platform.

- **2.6: Arrangements of Electrons** by Anonymous is licensed CC BY-NC-SA 3.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

2.5: The Periodic Table

Learning Objectives

- Explain how elements are organized into the periodic table.
- Describe how some characteristics of elements relate to their positions on the periodic table.

In the 19th century, many previously unknown elements were discovered, and scientists noted that certain sets of elements had similar chemical properties. For example, chlorine, bromine, and iodine react with other elements (such as sodium) to make similar compounds. Likewise, lithium, sodium, and potassium react with other elements (such as oxygen) to make similar compounds. Why is this so?

In 1864, Julius Lothar Meyer, a German chemist, organized the elements by atomic mass and grouped them according to their chemical properties. Later that decade, Dmitri Mendeleev, a Russian chemist, organized all the known elements according to similar properties. He left gaps in his table for what he thought were undiscovered elements, and he made some bold predictions regarding the properties of those undiscovered elements. When elements were later discovered whose properties closely matched Mendeleev's predictions, his version of the table gained favor in the scientific community. Because certain properties of the elements repeat on a regular basis throughout the table (that is, they are periodic), it became known as the periodic table.

> *Mendeleev had to list some elements out of the order of their atomic masses to group them with other elements that had similar properties.*

The periodic table is one of the cornerstones of chemistry because it organizes all the known elements on the basis of their chemical properties. A modern version is shown in Figure **2.5.1**. Most periodic tables provide additional data (such as atomic mass) in a box that contains each element's symbol. The elements are listed in order of atomic number.

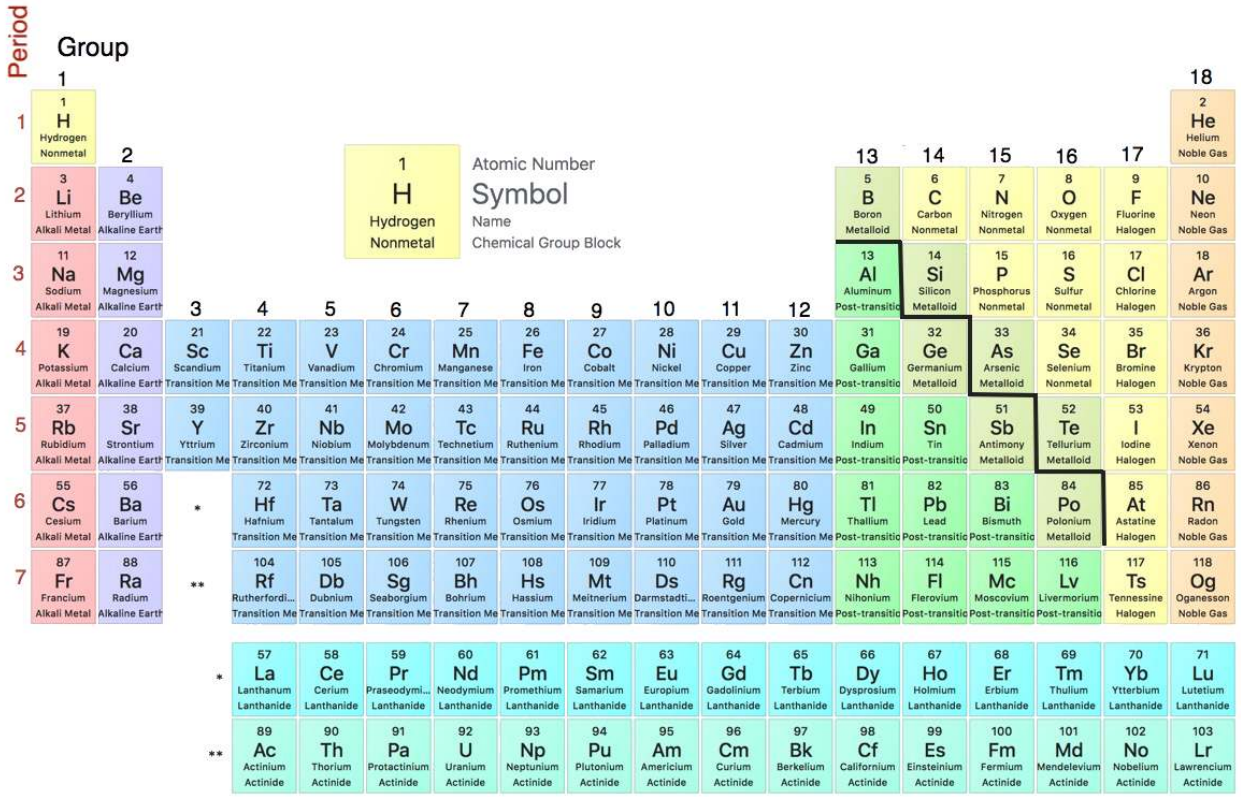


Figure **2.5.1**: Modern Periodic Table. (Public Domain; PubChem modified Leticia Colmenares).

Features of the Periodic Table

Elements that have similar chemical properties are grouped in columns called **groups** (or families). As well as being numbered, some of these groups have names—for example, *alkali metals* (the first column of elements), *alkaline earth metals* (the second column of elements), *halogens* (the next-to-last column of elements), and *noble gases* (the last column of elements).

Each row of elements on the periodic table is called a **period**. Periods have different lengths; the first period has only 2 elements (hydrogen and helium), while the second and third periods have 8 elements each. The fourth and fifth periods have 18 elements each, and later periods are so long that a segment from each is removed and placed beneath the main body of the table.

Metals, Nonmetals and Metalloids

Certain elemental properties become apparent in a survey of the periodic table as a whole. Every element can be classified as either a metal, a nonmetal, or a semimetal, as shown in Figure **2.5.2**. A metal is a substance that is shiny, typically (but not always) silvery in color, and an excellent conductor of electricity and heat. Metals are also malleable (they can be beaten into thin sheets) and ductile (they can be drawn into thin wires). A nonmetal is typically dull and a poor conductor of electricity and heat. Solid nonmetals are also very brittle. As shown in Figure **2.5.2**, **metals** occupy the left three-fourths of the periodic table, while **nonmetals** (except for hydrogen) are clustered in the upper right-hand corner of the periodic table. The elements with properties intermediate between those of metals and nonmetals are called **semimetals** (or **metalloids**). Elements adjacent to the **bold zigzag** line in the right-hand portion of the periodic table have semimetal properties.

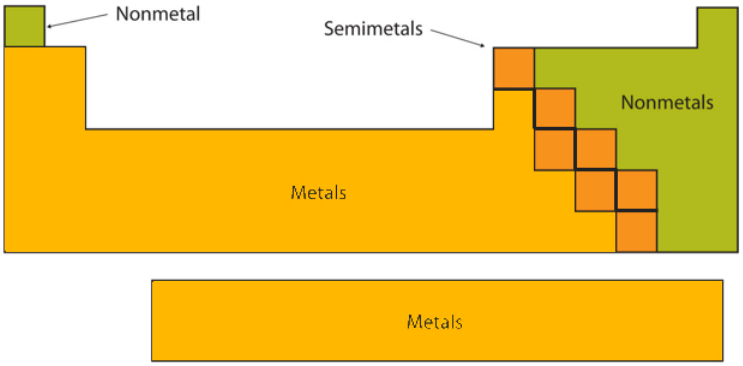


Figure **2.5.2**: Types of Elements. Elements are either metals, nonmetals, or semimetals. Each group is located in a different part of the periodic table.

Example 2.5.1

Based on its position in the periodic table, do you expect selenium (Se) to be a metal, a nonmetal, or a semimetal?

Solution

The atomic number of selenium is 34, which places it in period 4 and group 16. In Figure 2.7.1, selenium lies above and to the right of the diagonal line marking the boundary between metals and nonmetals, so it should be a nonmetal. Note, however, that because selenium is close to the metal-nonmetal dividing line, it would not be surprising if selenium were similar to a semimetal in some of its properties.

2.5.1 Exercise

Based on its location in the periodic table, do you expect indium (In) to be a nonmetal, a metal, or a semimetal?

Answer

metal

Representative, Transition and Inner-transition

Another way to categorize the elements of the periodic table is shown in Figure **2.5.3**. The first two columns on the left and the last six columns on the right are called the **main group** or **representative** elements. The ten-column block between these columns contains the **transition metals**. The two rows beneath the main body of the periodic table contain the inner transition metals. The elements in these two rows are also referred to as, respectively, the **lanthanide metals** and the **actinide metals**.

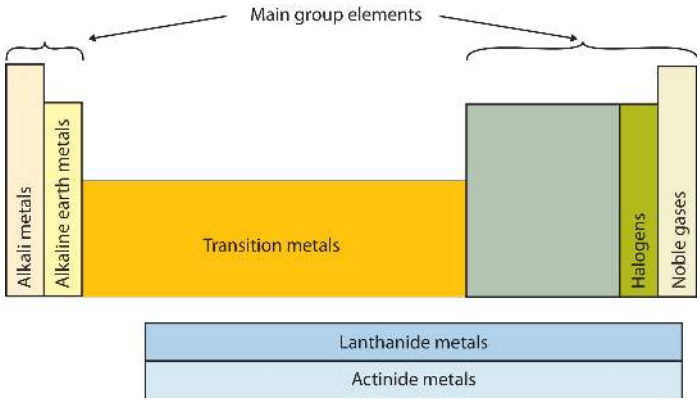


Figure **2.5.3**: Special Names for Sections of the Periodic Table. Some sections of the periodic table have special names. The elements lithium, sodium, potassium, rubidium, cesium, and francium are collectively known as alkali metals.

Alkali metals are the first column. Alkaline earth metals are the second. Halogens are the second to last column. Noble gases are the last column.

To Your Health: Transition Metals in the Body

Most of the elemental composition of the human body consists of main group elements. The first element appearing on the list that is not a main group element is iron, at 0.006 percentage by mass. Because iron has relatively massive atoms, it would appear even lower on a list organized in terms of percent by *atoms* rather than percent by mass.

Iron is a transition metal. Transition metals have interesting chemical properties, partially because some of their electrons are in *d* subshells. The chemistry of iron makes it a key component in the proper functioning of red blood cells.

Red blood cells are cells that transport oxygen from the lungs to cells of the body and then transport carbon dioxide from the cells to the lungs. Without red blood cells, animal respiration as we know it would not exist. The critical part of the red blood cell is a protein called *hemoglobin*. Hemoglobin combines with oxygen and carbon dioxide, transporting these gases from one location to another in the body. Hemoglobin is a relatively large molecule, with a mass of about 65,000 u.

The crucial atom in the hemoglobin protein is iron. Each hemoglobin molecule has four iron atoms, which act as binding sites for oxygen. It is the presence of this particular transition metal in your red blood cells that allows you to use the oxygen you inhale.

Other transition metals have important functions in the body, despite being present in low amounts. Zinc is needed for the body's immune system to function properly, as well as for protein synthesis and tissue and cell growth. Copper is also needed for several proteins to function properly in the body. Manganese is needed for the body to metabolize oxygen properly. Cobalt is a necessary component of vitamin B-12, a vital nutrient. These last three metals are not listed explicitly in Table 2.1.2, so they are present in the body in very small quantities. However, even these small quantities are required for the body to function properly.

As previously noted, the periodic table is arranged so that elements with similar chemical behaviors are in the same group. Chemists often make general statements about the properties of the elements in a group using descriptive names with historical origins. For example, the elements of Group 1 are known as the alkali metals, Group 2 are the alkaline earth metals, Group 17 are the halogens, and Group 18 are the noble gases.

Group 1: The Alkali Metals

The alkali metals are lithium, sodium, potassium, rubidium, cesium, and francium. Hydrogen is unique in that it is generally placed in Group 1, but it is not a metal. The compounds of the alkali metals are common in nature and daily life. One example is table salt (sodium chloride); lithium compounds are used in greases, in batteries, and as drugs to treat patients who exhibit manic-depressive, or bipolar, behavior. Although lithium, rubidium, and cesium are relatively rare in nature, and francium is so unstable and highly radioactive that it exists in only trace amounts, sodium and potassium are the seventh and eighth most abundant elements in Earth's crust, respectively.

Group 2: The Alkaline Earth Metals

The alkaline earth metals are beryllium, magnesium, calcium, strontium, barium, and radium. Beryllium, strontium, and barium are rare, and radium is unstable and highly radioactive. In contrast, calcium and magnesium are the fifth and sixth most abundant elements on Earth, respectively; they are found in huge deposits of limestone and other minerals.

Group 17: The Halogens

The halogens are fluorine, chlorine, bromine, iodine, and astatine. The name halogen is derived from the Greek words for "salt forming," which reflects that all the halogens react readily with metals to form compounds, such as sodium chloride and calcium chloride (used in some areas as road salt).

Compounds that contain the fluoride ion are added to toothpaste and the water supply to prevent dental cavities. Fluorine is also found in Teflon coatings on kitchen utensils. Although chlorofluorocarbon propellants and refrigerants are believed to lead to the depletion of Earth's ozone layer and contain both fluorine and chlorine, the latter is responsible for the adverse effect on the ozone layer. Bromine and iodine are less abundant than chlorine, and astatine is so radioactive that it exists in only negligible amounts in nature.

Group 18: The Noble Gases

The noble gases are helium, neon, argon, krypton, xenon, and radon. Because the noble gases are composed of only single atoms, they are called monatomic. At room temperature and pressure, they are **unreactive gases**. Because of their lack of reactivity, for many years they were called **inert gases** or rare gases. However, the first chemical compounds containing the noble gases were prepared in 1962. Although the noble gases are relatively minor constituents of the atmosphere, natural gas contains substantial amounts of helium. Because of its low reactivity, argon is often used as an unreactive (inert) atmosphere for welding and in light bulbs. The red light emitted by neon in a gas discharge tube is used in neon lights.

To Your Health: Radon

Radon is an invisible, odorless noble gas that is slowly released from the ground, particularly from rocks and soils whose uranium content is high. Because it is a noble gas, radon is not chemically reactive. Unfortunately, it is radioactive, and increased exposure to it has been correlated with an increased lung cancer risk.

Because radon comes from the ground, we cannot avoid it entirely. Moreover, because it is denser than air, radon tends to accumulate in basements, which if improperly ventilated can be hazardous to a building's inhabitants. Fortunately, specialized ventilation minimizes the amount of radon that might collect. Special fan-and-vent systems are available that draw air from below the basement floor, before it can enter the living space, and vent it above the roof of a house.

After smoking, radon is thought to be the second-biggest *preventable* cause of lung cancer in the United States. The American Cancer Society estimates that 10% of all lung cancers are related to radon exposure. There is uncertainty regarding what levels of exposure cause cancer, as well as what the exact causal agent might be (either radon or one of its breakdown products, many of which are also radioactive and, unlike radon, not gases). The US Environmental Protection Agency recommends testing every floor below the third floor for radon levels to guard against long-term health effects.

Why do elements in a given group have similar properties?

The periodic table is organized on the basis of similarities in elemental properties, but what explains these similarities? It turns out that the shape of the periodic table reflects the filling of subshells with electrons, as shown in Figure **2.5.4**. Starting with the first

period and going from left to right, the table reproduces the order of filling of the electron subshells in atoms. Furthermore, elements in the same *group* share the same valence shell electron configuration. For example, all elements in the first column have a single *s* electron in their valence shells, so their electron configurations can be described as ns^1 (where *n* represents the shell number). This last observation is crucial. Chemistry is largely the result of interactions between the valence electrons of different atoms. Thus, atoms that have **the same valence shell electron configuration** will have **similar chemistry.**

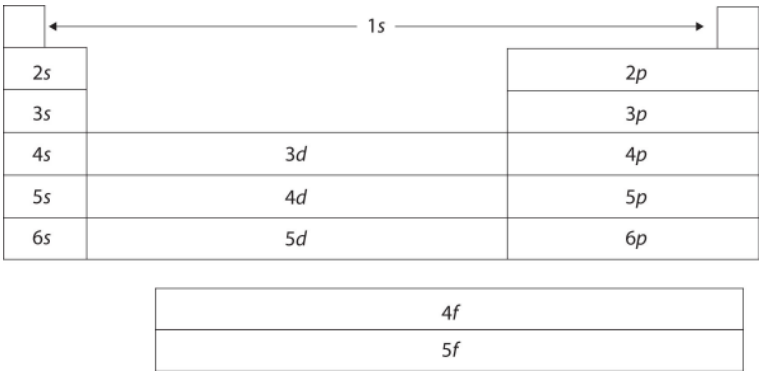


Figure **2.5.4** The Shape of the Periodic Table. The shape of the periodic table reflects the order in which electron shells and subshells fill with electrons.

Example 2.5.1

Using the variable *n* to represent the number of the valence electron shell, write the valence shell electron configuration for each group.

a. the alkaline earth metals
b. the column of elements headed by carbon

Answer a

The alkaline earth metals are in the second column of the periodic table. This column corresponds to the *s* subshell being filled with 2 electrons. Therefore, the valence shell electron configuration is ns^2.

Answer b

The electron configuration of carbon is $1s^22s^22p^2$. Its valence shell electron configuration is $2s^22p^2$. Every element in the same column should have a similar valence shell electron configuration, which we can represent as ns^2np^2.

Exercise 2.5.1

Using the variable *n* to represent the number of the valence electron shell, write the valence shell electron configuration for each group.

a. the halogens
b. the column of elements headed by oxygen

Answer a

The halogens are in the 17th column (or Group 7A) of the periodic table. This column corresponds to the *p* subshell being filled with 5 electrons. Therefore, the valence shell electron configuration is ns^2np^5.

Answer b

The column headed by O is the 16th column (or Group 6A). This column corresponds to the *p* subshell being filled with 4 electrons. Therefore, the valence shell electron configuration is ns^2np^4.

Valence Electrons and Group Number

The number of valence electrons of an element can be determined by the periodic table group (vertical column) in which the element is categorized. With the exception of groups 3–12 (the transition metals), the units digit of the group number identifies how many valence electrons are associated with a neutral atom of an element listed under that particular column.

Table **2.5.1**. The Group number and the number of valence electrons.

Periodic table group	Valence electrons
Group 1 (I) (alkali metals)	1
Group 2 (II) (alkaline earth metals)	2
Groups 3-12 (transition metals)	2*
Group 13 (III) (boron group)	3
Group 14 (IV) (carbon group)	4
Group 15 (V) (pnictogens)	5
Group 16 (VI) (chalcogens)	6
Group 17 (VII) (halogens)	7
Group 18 (VIII or 0) (noble gases)	8**

** The general method for counting valence electrons is generally not useful for transition metals.*

*** Except for helium, which has only two valence electrons.*

Atomic Radius

The periodic table is useful for understanding atomic properties that show periodic trends. One such property is the atomic radius (Figure **2.5.5**). The atomic radius is defined as one-half the distance between the nuclei of identical atoms that are bonded together. The units for atomic radii are picometers, equal to 10^{-12} meters. As an example, the internuclear distance between the two hydrogen atoms in an H_2 molecule is measured to be $74\ pm$. Therefore, the atomic radius of a hydrogen atom is $\frac{74}{2} = 37\ pm$.

As mentioned earlier, the higher the shell number, the farther from the nucleus the electrons in that shell are likely to be. In other words, the size of an atom is generally determined by the number of the valence electron shell. Therefore, as we go down a column on the periodic table, the atomic radius increases. As we go *across* a period on the periodic table, however, electrons are being added to the *same* valence shell; meanwhile, more protons are being added to the nucleus, so the positive charge of the nucleus is increasing. The increasing positive charge attracts the electrons more strongly, pulling them closer to the nucleus. Consequently, as we go across a period, from left to right, the atomic radius decreases. These trends are seen clearly in Figure **2.5.5**

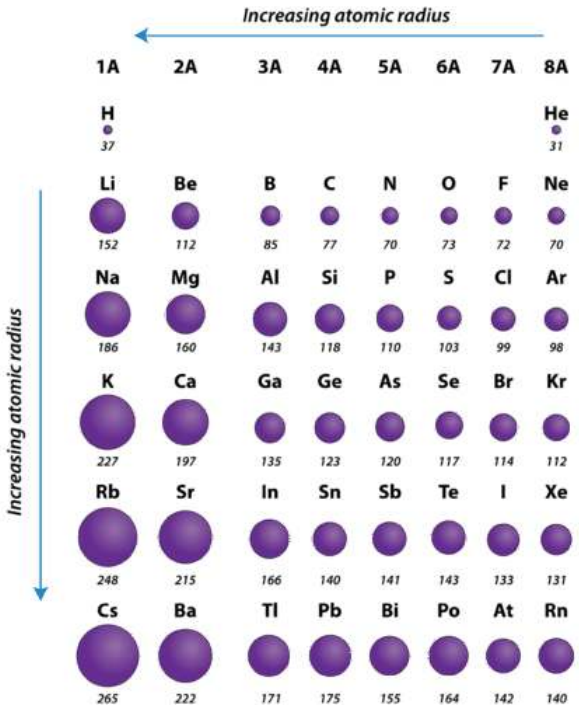


Figure **2.5.5** Trends on the Periodic Table. Atomic radii of the representative elements measured in picometers. The relative sizes of the atoms show several trends with regard to the structure of the periodic table. Atoms become larger going down a group and going from right to left across a period.

✔ Example 2.5.2

Using the periodic table (rather than Figure **2.5.5**), which atom is larger?

a. N or Bi
b. Mg or Cl

Answer a

Bi is below N in Group 5A in the periodic table and has electrons in higher-numbered shells, hence we expect that Bi atoms are larger than N atoms.

Answer b

Both Mg and Cl are in period 3 of the periodic table, but Cl lies farther to the right. Therefore we expect Mg atoms to be larger than Cl atoms.

? Exercise 2.5.2

Using the periodic table (rather than Figure **2.5.5**), which atom is larger?

a. Li or F
b. Na or K

Answer a

Li and F are on the same period, but F lies farther to the right. Therefore, we expect Li to be larger than F atoms.

Answer b

K lies below Na in Group 1A, hence has more electron shells, making it larger than Na.

Career Focus: Clinical Chemist

Clinical chemistry is the area of chemistry concerned with the analysis of body fluids to determine the health status of the human body. Clinical chemists measure a variety of substances, ranging from simple elements such as sodium and potassium to complex molecules such as proteins and enzymes, in blood, urine, and other body fluids. The absence or presence, or abnormally low or high amounts, of a substance can be a sign of some disease or an indication of health. Many clinical chemists use sophisticated equipment and complex chemical reactions in their work, so they not only need to understand basic chemistry, but also be familiar with special instrumentation and how to interpret test results.

Concept Review Exercises

1. How are the elements organized into the periodic table?
2. Looking at the periodic table, where do the following elements appear?
    a. the metals
    b. the nonmetals
    c. the halogens
    d. the transition metals
    e. the noble gases
3. Describe the trends in atomic radii as related to an element's position on the periodic table.

Answers

1. Elements are organized in order of increasing atomic number.
2. a. the left three-quarters of the periodic table (to the left of the zigzag band)
    b. the right quarter of the periodic table (to the right of the zigzag band)
    c. the next-to-last column of the periodic table
    d. the middle section of the periodic table
    e. the last column of the periodic table
3. As you go across the periodic table, atomic radii decrease; as you go down the periodic table, atomic radii increase.

Key Takeaways

- The chemical elements are arranged in a chart called the periodic table.
- Some characteristics of the elements are related to their position on the periodic table.
- The number of valence electrons of an element can be determined by the group (vertical column) number in the Periodic Table. Elements with the same number of valence electrons have similar chemical properties.

This page titled 2.5: The Periodic Table is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous via source content that was edited to the style and standards of the LibreTexts platform.

- **2.7: The Periodic Table** by Anonymous is licensed CC BY-NC-SA 3.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

2.6: Health Connections- Essential Elements for Life

Learning Objective

- To understand the importance of elements to nutrition.

Of the approximately 115 elements known, only the 19 highlighted in purple in Figure **2.6.1** are absolutely required in the human diet. These elements—called essential elements—are restricted to the first four rows of the periodic table, with only two or three exceptions (molybdenum, iodine, and possibly tin in the fifth row). Some other elements are essential for specific organisms. For example, boron is required for the growth of certain plants, bromine is widely distributed in marine organisms, and tungsten is necessary for some microorganisms.

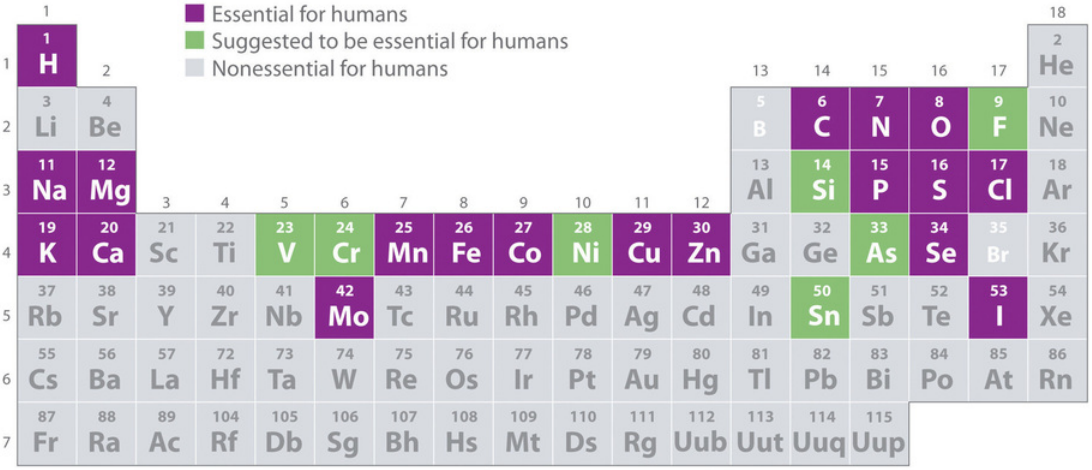


Figure **2.6.1**: The Essential Elements in the Periodic Table. Elements that are known to be essential for human life are shown in purple; elements that are suggested to be essential are shown in green. Elements not known to be essential are shown in gray.

What makes an element “essential”? By definition, an essential element is one that is required for life and whose absence results in death. Because of the experimental difficulties involved in producing deficiencies severe enough to cause death, especially for elements that are required in very low concentrations in the diet, a somewhat broader definition is generally used. An element is considered to be essential if a deficiency consistently causes abnormal development or functioning and if dietary supplementation of that element—and only that element—prevents this adverse effect. Scientists determine whether an element is essential by raising rats, chicks, and other animals on a synthetic diet that has been carefully analyzed and supplemented with acceptable levels of all elements except the element of interest (E). Ultraclean environments, in which plastic cages are used and dust from the air is carefully removed, minimize inadvertent contamination. If the animals grow normally on a diet that is as low as possible in E, then either E is not an essential element or the diet is not yet below the minimum required concentration. If the animals do not grow normally on a low-E diet, then their diets are supplemented with E until a level is reached at which the animals grow normally. This level is the minimum required intake of element E.

Classification of the Essential Elements

The approximate elemental composition of a healthy 70.0 kg (154 lb) adult human is listed in Table **2.6.1**. Note that most living matter consists primarily of the so-called bulk elements: oxygen, carbon, hydrogen, nitrogen, and sulfur—the building blocks of the compounds that constitute our organs and muscles. These five elements also constitute the bulk of our diet; tens of grams per day are required for humans. Six other elements—sodium, magnesium, potassium, calcium, chlorine, and phosphorus—are often referred to as macrominerals because they provide essential ions in body fluids and form the major structural components of the body. In addition, phosphorus is a key constituent of both DNA and RNA: the genetic building blocks of living organisms. The six macrominerals are present in the body in somewhat smaller amounts than the bulk elements, so correspondingly lower levels are required in the diet. The remaining essential elements—called trace elements—are present in very small amounts, ranging from a few grams to a few milligrams in an adult human. Finally, measurable levels of some elements are found in humans but are not required for growth or good health. Examples are rubidium and strontium, whose chemistry is similar to that of the elements

immediately above them in the periodic table (potassium and calcium, respectively, which are essential elements). Because the body's mechanisms for extracting potassium and calcium from foods are not 100% selective, small amounts of rubidium and strontium, which have no known biological function, are absorbed.

Table **2.6.1**: Approximate Elemental Composition of a Typical 70 kg Human

Bulk Elements (kg)		Macrominerals (g)	
oxygen	44	calcium	1700
carbon	12.6	phosphorus	680
hydrogen	6.6	potassium	250
nitrogen	1.8	chlorine	115
sulfur	0.1	sodium	70
		magnesium	42
Trace Elements (mg)			
iron	5000	lead	35
silicon	3000	barium	21
zinc	1750	molybdenum	14
rubidium	360	boron	14
copper	280	arsenic	~3
strontium	280	cobalt	~3
bromine	140	chromium	~3
tin	140	nickel	~3
manganese	70	selenium	~2
iodine	70	lithium	~2
aluminum	35	vanadium	~2

The Trace Elements

Because it is difficult to detect low levels of some essential elements, the trace elements were relatively slow to be recognized as essential. Iron was the first. In the 17th century, anemia was proved to be caused by an iron deficiency and often was cured by supplementing the diet with extracts of rusty nails. It was not until the 19th century, however, that trace amounts of iodine were found to eliminate goiter (an enlarged thyroid gland). This is why common table salt is "iodized": a small amount of iodine is added. Copper was shown to be essential for humans in 1928, and manganese, zinc, and cobalt soon after that. Molybdenum was not known to be an essential element until 1953, and the need for chromium, selenium, vanadium, fluorine, and silicon was demonstrated only in the last 50 years. It seems likely that in the future other elements, possibly including tin, will be found to be essential at very low levels.

Many compounds of trace elements, such as arsenic, selenium, and chromium, are toxic and can even cause cancer, yet these elements are identified as essential elements in Figure **2.6.1**. In fact, there is some evidence that one bacterium has replaced phosphorus with arsenic, although the finding is controversial. This has opened up the possibility of a "shadow biosphere" on Earth in which life evolved from an as yet undetected common ancestor. How can elements toxic to life be essential? First, the toxicity of an element often depends on its chemical form—for example, only certain compounds of chromium are toxic, whereas others are used in mineral supplements. Second, as shown in Figure **2.6.2**, every element has three possible levels of dietary intake: deficient, optimum, and toxic in order of increasing concentration in the diet. Very low intake levels lead to symptoms of deficiency. Over

some range of higher intake levels, an organism is able to maintain its tissue concentrations of the element at a level that optimizes biological functions. Finally, at some higher intake level, the normal regulatory mechanisms are overloaded, causing toxic symptoms to appear. Each element has its own characteristic curve. Both the width of the plateau and the specific concentration corresponding to the center of the plateau region differ by as much as several orders of magnitude for different elements. In the adult human, for example, the recommended daily dietary intake is 10–18 mg of iron, 2–3 mg of copper, and less than 0.1 mg of chromium and selenium.

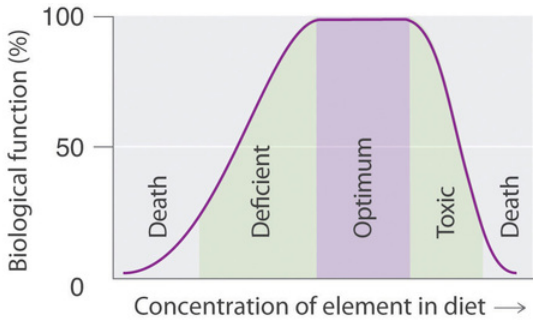


Figure **2.6.2**: Possible Concentrations of an Essential Element in the Diet. The deficient, optimum, and toxic concentrations are different for different elements.

Amplification

How can elements that are present in such minuscule amounts have such large effects on an organism's health? Our knowledge of the pathways by which each of the known trace elements affects health is far from complete, but certain general features are clear. The trace elements participate in an amplification mechanism; that is, they are essential components of larger biological molecules that are capable of interacting with or regulating the levels of relatively large amounts of other molecules. For example, vitamin B_{12} contains a single atom of cobalt, which is essential for its biological function. If the molecule whose level is controlled by the trace element can regulate the level of another molecule, and more and more molecules, then the potential exists for extreme amplification of small variations in the level of the trace element. One goal of modern chemical research is to elucidate in detail the roles of the essential elements. In subsequent chapters, we will introduce some results of this research to demonstrate the biological importance of many of the elements and their compounds.

Summary

About 19 of the approximately 115 known elements are essential for humans. An essential element is one whose absence results in abnormal biological function or development that is prevented by dietary supplementation with that element. Living organisms contain relatively large amounts of oxygen, carbon, hydrogen, nitrogen, and sulfur (these five elements are known as the bulk elements), along with sodium, magnesium, potassium, calcium, chlorine, and phosphorus (these six elements are known as macrominerals). The other essential elements are the trace elements, which are present in very small quantities. Dietary intakes of elements range from deficient to optimum to toxic with increasing quantities; the optimum levels differ greatly for the essential elements.

This page titled 2.6: Health Connections- Essential Elements for Life is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous.

- **1.9: Essential Elements for Life** by Anonymous is licensed CC BY-NC-SA 3.0.

2.7: Case Study- Electrons and Electronic Structure in Medical Applications

Scenario: Dr. Sarah Thompson, a seasoned radiologist, meets with John, a patient who has been diagnosed with an early-stage, localized form of cancer. Dr. Thompson sits down with John and his family to discuss the proposed treatment plan—radiation therapy. She carefully explains how this therapy uses the principles of electron behavior and atomic structure to target cancer cells with high precision while sparing the surrounding healthy tissue.

Electrons and Electronic Structure: At the heart of Dr. Thompson's explanation is the concept that each atom, the fundamental building block of matter, is made up of a nucleus and electrons. The electrons are arranged in layers or shells around the nucleus, and their specific arrangement is referred to as the electronic structure. This structure dictates how an atom will interact with radiation.

Application in Radiation Therapy: Radiation therapy, Dr. Thompson explains to John, works by sending high-energy particles or waves through the body to the cancer cells. These particles or waves are absorbed by the electrons in the DNA of the cells, causing ionization. In other words, the electrons are knocked out of their orbits, leading to DNA damage. Because their rapid division rate makes cancer cells more vulnerable to this damage, they are preferentially destroyed over healthy cells.

Case Study Questions:

1. **How does electron movement affect DNA structure and function?**
2. **How can knowledge of electron configuration impact medical treatments?**

Hands-on Classroom Activities:

1. **Build a Model:** In this activity, students are tasked with constructing three-dimensional models that represent the arrangement of electron shells and valence electrons. Using materials such as colored balls and sticks, they will assemble structures that mimic the atomic framework, providing a tangible way to comprehend the abstract concepts of atomic structure and electron distribution. This hands-on project aims to deepen students' understanding of how electrons influence chemical bonding and molecular formation.
2. **Research Discussion:** Following the model-building exercise, students will engage in a research discussion centered on the latest developments in radiation therapy. They will investigate and analyze scholarly articles and clinical studies that examine the critical role of electron behavior in advancing therapeutic techniques. Each student or group is expected to present a summary of their research to the class, sparking an in-depth dialogue about the practical implications and potential innovations in the field of medical treatment.

Conclusion: As Dr. Thompson outlines the treatment plan, she reassures John that the approach is rooted in a deep scientific understanding of atomic behavior, specifically the interactions involving electrons. This case exemplifies how intricate knowledge of atomic and subatomic particles is not just an abstract scientific principle but a vital tool in the fight against cancer. It provides a beacon of hope for patients like John, highlighting the marriage of theoretical science with practical, life-saving medical interventions.

2.7: Case Study- Electrons and Electronic Structure in Medical Applications is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

2.8: 3D Printing Activity - Periodic Trends

Sometimes it can be challenging to visualize the periodic trends the first time students learn about them. Creating tactile 3-dimensional periodic tables can allow for better understanding of these trends.

For this activity, the instructor will print out the three-dimensional periodic tables before class and pass them around your class while discussing periodic trends. The periodic tables can be reused in future years once they have been printed.

The .stl files for these periodic tables are available in the supporting information of the following publication: *Journal of Chemical Education* **2019**, *96*, 285-290, DOI: 10.1021/acs.jchemed.8b00592 (https://pubs.acs.org/doi/abs/10.1021/acs.jchemed.8b00592). The manuscript was written by Dr. Bob LeSuer of SUNY Brockport. The specific file to download is the last supplementary zipped file: “ed8b00592_si_004.zip”. Within this zip file are several options, including multiple sizes of atomic radius, ionization energy, and electron affinity, and electronegativity trends, among others.

2.8: 3D Printing Activity - Periodic Trends is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

2.E: Exercises

Multiple-Choice Questions

1. Which of the following has a positive charge?
    a. A proton
    b. An electron
    c. A neutron
    d. A hydrogen atom
2. Which of the following is the mass number for ^{79}Br?
    a. 35
    b. 44
    c. 79
    d. 79.904
3. How many electrons are present in Mg^{2+}?
    a. 10
    b. 12
    c. 14
    d. 24
4. Which of the following is the correct set of protons, neutrons, and electrons for $^{113}Cd^{2+}$?
    a. 48, 65, 48
    b. 48, 65, 50
    c. 48, 65, 46
    d. 50, 65, 48
5. Which of the following is the correct chemical symbol for copper?
    a. C
    b. Co
    c. Cr
    d. Cu
6. Select the correct atomic symbol for an isotope of nitrogen with 8 neutrons.
    a. ^{7}N
    b. ^{8}N
    c. ^{14}N
    d. ^{15}N
7. The average atomic mass of chlorine is 35.4527 amu. There are two stable isotopes of chlorine: ^{35}Cl and ^{37}Cl. Given this information, which of the statements below is true?
    a. The fractional abundance of ^{35}Cl is greater than that of ^{37}Cl.
    b. The fractional abundance of ^{37}Cl is greater than that of ^{35}Cl.

c. The fractional abundances of ^{35}Cl and ^{37}Cl are equal.

d. The relative fractional abundances of ^{35}Cl and ^{37}Cl cannot be determined from this information.

8. How many valence electrons does an atom of phosphorus have?

a. 3

b. 5

c. 8

d. 15

9. To achieve an octet in its valence shell, sulfur must …

a. gain one electron

b. lose one electron

c. gain two electrons

d. lose two electrons

10. Based on your knowledge of the periodic variation in atomic size, which of the following correctly orders the elements in terms of decreasing atomic radius?

a. B, N, F

b. F, N, B

c. Li, K, Cs

d. K, Li, Cs

Warm-up Problems

1. Provide the name of the element associated with each of the following chemical symbols.

a. K

b. C

c. Ba

d. Al

2. Provide the chemical symbol for each of the following elements.

a. sodium

b. calcium

c. selenium

d. neon

3. How many protons, neutrons, and electrons are present in a $^{31}P^{3-}$ ion?

4. How many protons, neutrons, and electrons are present in a $^{7}Li^{+}$ ion?

5. Write the chemical symbol for the ion that has 16 protons, 18 neutrons, and 18 electrons.

6. Write the chemical symbol for the ion that has 11 protons, 12 neutrons, and 10 electrons.

7. How many valence electrons does a carbon atom have?

8. How many valence electrons does a chlorine atom have?

9. For each pair of elements, select the element with a **larger** atomic radius.

a. Na, Mg

b. F, Cl

c. P, O

10. For each pair of elements, select the element with a **larger** ionization energy.

a. Na, Mg

b. F, Cl

c. P, O

11. Order the following elements in terms of decreasing atomic radius: krypton, arsenic, phosphorus, chlorine.

12. Order the following elements in terms of increasing metallic character: fluorine, lithium, cesium, bromine.

Problems

1. The average atomic mass of iridium is 192.217 amu. This element has two stable isotopes: ^{191}Ir and ^{193}Ir. Based on the average atomic mass, explain which isotope has a larger fractional abundance.

2. The element potassium has an average atomic mass of 39.0983 amu. This element has three stable isotopes: K-39, K-40, and K-41.

a. Which of these isotopes has 21 neutrons?

b. Which of these isotopes has the largest fractional abundance? Explain your answer.

c. A single atom of potassium will never have a mass of 39.0983 amu. Explain why this is the case.

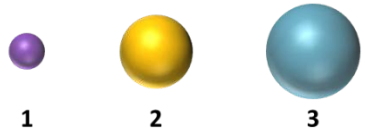
3. Which halogen is located in the same period as lithium?

4. Which alkaline earth metal is in the same period as silicon?

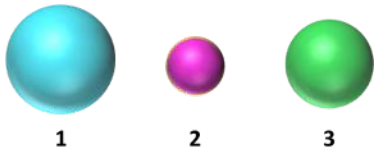
5. Is the ionization energy of chlorine larger or smaller than that of fluorine? Explain your answer.

6. Is the ionization energy of chlorine larger or smaller than that of silicon? Explain your answer.

7. Match the spheres shown in the image below with the elements: beryllium, carbon, oxygen.



8. Match the spheres shown in the image below with the elements: chlorine, bromine, iodine.



9. The elements phosphorus and oxygen are both classified as nonmetals. Which of these elements is considered more metallic? Explain your answer.

10. The elements rubidium and sodium are both classified as metals. Which of these elements is considered less metallic? Explain your answer.

Challenge Problem

1. When forming ionic bonds, atoms generally either donate or accept electrons in order to achieve a stable valence electron configuration. Explain whether fluorine is likely to donate or accept electrons when forming an ionic bond based on your knowledge of the octet rule and periodic trends.

Health-related Problems

1. Radioactive elements are used in medical imaging. For example, technetium-99 is made from molybdenum-99 and then used before it decays. How many protons, neutrons, and electrons are in technecium-99? Assume it has no charge.
2. Radioactive elements are used in medical imaging. For example, technetium-99 is made from molybdenum-99 and then used before it decays. How many protons, neutrons, and electrons are in molybdenum-99? Assume it has no charge.
3. One common ion inside the body is Mg^{2+}, the most stable form of magnesium under biological conditions. What group is this element in?
4. One common ion inside the body is Ca^{2+}, the most stable form of calcium under biological conditions. What group is this element in?
5. Positron Emission Tomography (PET) scans use a radioactive tracer for imaging. Fluorine-18 is a radioactive isotope used in some PET scans. How many protons, neutrons and electrons does it have if the element has a –1 charge?
6. Positron Emission Tomography (PET) scans use a radioactive tracer for imaging. Carbon-11 is a radioactive isotope used in some PET scans. How many protons, neutrons and electrons does it have if the element has a -2 charge?

2.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

3: Ionic and Covalent Compounds

Learning Objectives

- Outline the historical development of chemistry
- Provide examples of the importance of chemistry in everyday life
- Describe the scientific method and informs the scientific process
- Differentiate among hypotheses, theories, and laws
- Provide examples illustrating macroscopic, microscopic, and symbolic domains

Throughout human history, people have tried to convert matter into more useful forms. Our Stone Age ancestors chipped pieces of flint into useful tools and carved wood into statues and toys. These endeavors involved changing the shape of a substance without changing the substance itself. But as our knowledge increased, humans began to change the composition of the substances as well—clay was converted into pottery, hides were cured to make garments, copper ores were transformed into copper tools and weapons, and grain was made into bread.

Humans began to practice chemistry when they learned to control fire and use it to cook, make pottery, and smelt metals. Subsequently, they began to separate and use specific components of matter. A variety of drugs such as aloe, myrrh, and opium were isolated from plants. Dyes such as indigo and Tyrian purple were extracted from plant and animal matter. Metals were combined to form alloys—for example, copper and tin were combined to make bronze—and more elaborate smelting techniques produced iron. Alkalis were extracted from ashes, and soaps were prepared by combining these alkalis with fats. Alcohol was produced by fermentation and purified by distillation.

Attempts to understand the behavior of matter extend back more than 2500 years. As early as the sixth century BC, Greek philosophers discussed a system where water was the basis of everything. You may have heard of the Greek postulate that matter consists of four elements: earth, air, fire, and water. Subsequently, an amalgamation of chemical technologies and philosophical speculations was spread from Egypt, China, and the eastern Mediterranean by alchemists, who endeavored to transform “base metals” such as lead into “noble metals” such as gold and create elixirs to cure disease and extend life (Figure **3.1**).



Figure **3.1**: This portrayal shows an alchemist’s workshop circa 1580. Although alchemy made some useful contributions to how to manipulate matter, it was not scientific by modern standards. (credit: Chemical Heritage Foundation).

A sketch depicts 4 people stirring and handling chemicals. The chemicals are held in a variety of barrels and large cylinders. Several of the containers are being heated over burning embers. A large stove in the laboratory is filled with burning embers. There is also a large chest in the corner that is producing steam.

From alchemy came the historical progressions that led to modern chemistry: the isolation of drugs from natural sources, metallurgy, and the dye industry. Today, chemistry continues to deepen our understanding and improve our ability to harness and

control the behavior of matter. This effort has succeeded so well that many people do not realize either the central position of chemistry among the sciences or its importance and universality in daily life.

3.1: Chemistry: The Central Science

Chemistry is sometimes called “the central science” for its interconnectedness with many other STEM disciplines (STEM stands for areas of study in the science, technology, engineering, and math fields). Chemistry and the language of chemists play vital roles in biology, medicine, materials science, forensics, environmental science, and many other fields (Figure **3.2**). The basic principles of physics are essential for understanding many aspects of chemistry, and there is extensive overlap between many subdisciplines within the two fields, such as chemical physics and nuclear chemistry. Mathematics, computer science, and information theory provide important tools that help us calculate, interpret, describe, and generally make sense of the chemical world. Biology and chemistry converge in biochemistry, which is crucial to understanding the many complex factors and processes that keep living organisms (such as us) alive. Chemical engineering, materials science, and nanotechnology combine chemical principles and empirical findings to produce useful substances ranging from gasoline to fabrics to electronics. Agriculture, food science, veterinary science, brewing, and wine-making help provide sustenance in the form of food and drink to the world’s population. Medicine, pharmacology, biotechnology, and botany identify and produce substances that help keep us healthy. Environmental science, geology, oceanography, and atmospheric science incorporate many chemical ideas to help us better understand and protect our physical world. In astronomy and cosmology, chemical ideas are used to help understand the universe.

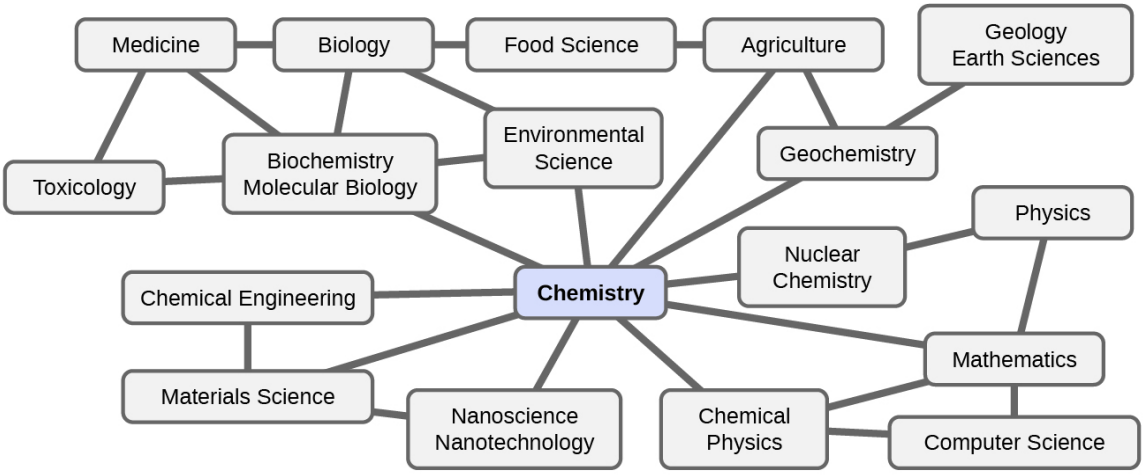


Figure **3.2**: Knowledge of chemistry is central to understanding a wide range of scientific disciplines. This diagram shows just some of the interrelationships between chemistry and other fields.

A flowchart shows a box containing chemistry at its center. Chemistry is connected to geochemistry, nuclear chemistry, chemical physics, nanoscience and nanotechnology, materials science, chemical engineering, biochemistry and molecular biology, environmental science, agriculture, and mathematics. Each of these disciplines is further connected to other related fields including medicine, biology, food science, geology earth sciences, toxicology, physics, and computer science.

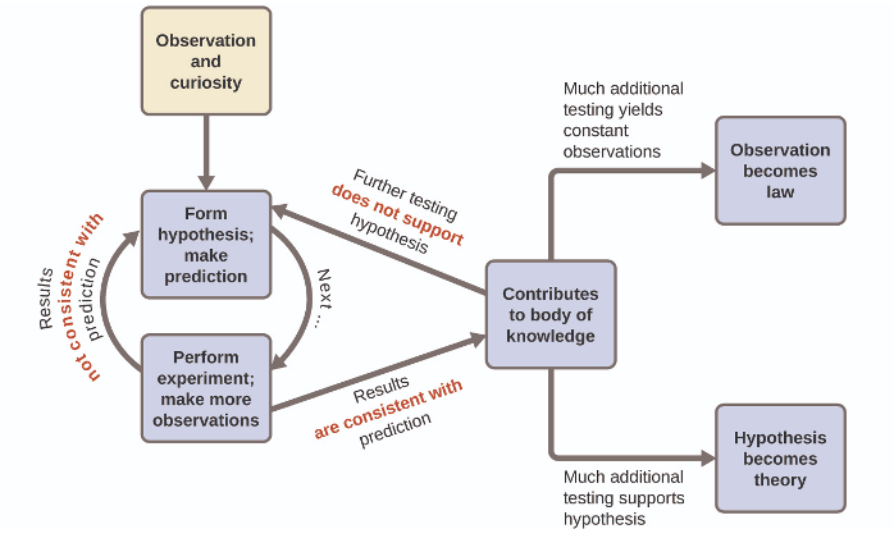
What are some changes in matter that are essential to daily life? Just a few examples are digesting and assimilating food; synthesizing polymers that are used to make clothing, containers, cookware, and credit cards; and refining crude oil into gasoline and other products. As you proceed through this course, you will discover many different examples of changes in the composition and structure of matter, how to classify these changes and how they occurred, their causes, the changes in energy that accompany them, and the principles and laws involved. As you learn about these things, you will be learning chemistry, the study of the composition, properties, and interactions of matter. The practice of chemistry is not limited to chemistry books or laboratories: It happens whenever someone is involved in changes in matter or in conditions that may lead to such changes.

3.2: The Scientific Method

Chemistry is a science based on observation and experimentation. Doing chemistry involves attempting to answer questions and explain observations in terms of the laws and theories of chemistry, using procedures accepted by the scientific community. There is no single route to answering a question or explaining an observation. However, one aspect is common to every approach: each uses knowledge based on experiments that can be reproduced to verify the results. Some routes involve a hypothesis, a tentative

explanation of observations that acts as a guide for gathering and checking information. We test a hypothesis by experimentation, calculation, and/or comparison with the experiments of others and then refine it as needed.

Some hypotheses are attempts to explain the behavior that is summarized in laws. The laws of science summarize a vast number of experimental observations and describe or predict some facet of the natural world. If such a hypothesis can explain a large body of experimental data, it can reach the status of a theory. Scientific theories are well-substantiated, comprehensive, testable explanations of particular aspects of nature. Theories are accepted because they provide satisfactory explanations but can be modified if new data becomes available. The path of discovery that leads from question and observation to law or hypothesis to theory, combined with experimental verification of the hypothesis and any necessary modification of the theory, is called the scientific method (Figure **3.3**).



In this flowchart, the observation and curiosity box has an arrow pointing to a box labeled "Form hypothesis; make prediction." A curved arrow labeled next connects this box to a box labeled "Perform experiment; make more observations." Another arrow points back to the box that says "Form hypothesis; make prediction." This arrow is labeled results not consistent with prediction. Another arrow, labeled "Results are consistent with prediction" points from the perform experiment box to a box labeled contributes to body of knowledge. However, an arrow also points from "Contributes to body of knowledge" back to the "Form hypothesis; make prediction" box. This arrow is labeled "Further testing does not support hypothesis." There are also two other arrows leading out from "Contributes to body of knowledge." One arrow is labeled "Much additional testing yields constant observations." This leads to the "Observation becomes law" box. The other arrow is labeled "Much additional testing supports hypothesis." This arrow leads to the "Hypothesis becomes theory" box.

Figure **3.3**: The scientific method follows a process similar to the one shown in this diagram. All the key components are shown, in roughly the right order. Scientific progress is seldom neat and clean: It requires open inquiry and the reworking of questions and ideas in response to findings.

3.3: The Domains of Chemistry

Chemists study and describe the behavior of matter and energy in three different domains: macroscopic, microscopic, and symbolic. These domains provide different ways of considering and describing chemical behavior.

Macro is a Greek word meaning “large.” The macroscopic domain is familiar to us: It is the realm of everyday things that are large enough to be sensed directly by human sight or touch. In daily life, this includes the food you eat and the breeze you feel on your face. The macroscopic domain also includes everyday and laboratory chemistry, where we observe and measure physical and chemical properties or changes such as density, solubility, and flammability.

The microscopic domain of chemistry is almost always visited in the imagination. *Micro* also comes from Greek and means “small.” Some aspects of the microscopic domains are visible through a microscope, such as a magnified image of graphite or bacteria. Viruses, for instance, are too small to be seen with the naked eye, but when we’re suffering from a cold, we’re reminded of how real they are.

However, most subjects in the microscopic domain of chemistry—such as atoms and molecules—are too small to be seen even with standard microscopes and often must be pictured in the mind. Other components of the microscopic domain include ions and

electrons, protons and neutrons, and chemical bonds, each of which is far too small to see. This domain includes the individual metal atoms in a wire, the ions that compose a salt crystal, the changes in individual molecules that result in a color change, the conversion of nutrient molecules into tissue and energy, and the evolution of heat as bonds that hold atoms together are created.

The symbolic domain contains the specialized language used to represent components of the macroscopic and microscopic domains. Chemical symbols (such as those used in the periodic table), chemical formulas, and chemical equations are part of the symbolic domain, as are graphs and drawings. We can also consider calculations as part of the symbolic domain. These symbols play an important role in chemistry because they help interpret the behavior of the macroscopic domain in terms of the components of the microscopic domain. One challenge for students learning chemistry is recognizing that the same symbols can represent different things in the macroscopic and microscopic domains, and one of the features that makes chemistry fascinating is the use of a domain that must be imagined to explain behavior in a domain that can be observed.

A helpful way to understand the three domains is via the essential and ubiquitous substance of water. That water is a liquid at moderate temperatures, will freeze to form a solid at lower temperatures, and boil to form a gas at higher temperatures (Figure 1.1.4) are macroscopic observations. But some properties of water fall into the microscopic domain—what we cannot observe with the naked eye. The description of water as comprised of two hydrogen atoms and one oxygen atom, and the explanation of freezing and boiling in terms of attractions between these molecules, is within the microscopic arena. The formula H_2O, which can describe water at either the macroscopic or microscopic levels, is an example of the symbolic domain. The abbreviations (*g*) for gas, (*s*) for solid, and (*l*) for liquid are also symbolic.

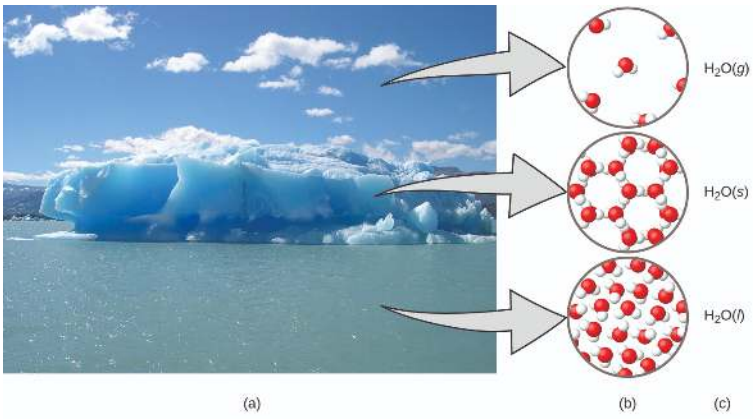


Figure **3.4**: (a) Moisture in the air, icebergs, and the ocean represent water in the macroscopic domain. (b) At the molecular level (microscopic domain), gas molecules are far apart and disorganized, solid water molecules are close together and organized, and liquid molecules are close together and disorganized. (c) The formula H_2O symbolizes water, and (g), (s), and (l) symbolize its phases. Note that clouds actually comprise either very small liquid water droplets or solid water crystals; gaseous water in our atmosphere is not visible to the naked eye, although it may be sensed as humidity. (Credit a: modification of work by "Gorkaazk"/Wikimedia Commons).

Figure A shows a photo of an iceberg floating in a sea has three arrows. Each arrow points to figure B, which contains three diagrams showing how the water molecules are organized in the air, ice, and sea. In the air, which contains the gaseous form of water, H subscript 2 O gas, the water molecules are disconnected and widely spaced. In the ice, which is the solid form of water, H subscript 2 O solid, the water molecules are bonded into rings, each containing six water molecules. Three of these rings are connected to each other. In the sea, which is the liquid form of water, H subscript 2 O liquid, the water molecules are very densely packed. The molecules are not bonded together.

3.4: Key Concepts and Summary

Chemistry deals with the composition, structure, and properties of matter, and the ways by which various forms of matter may be interconverted. Thus, it occupies a central place in the study and practice of science and technology. Chemists use the scientific method to perform experiments, pose hypotheses, and formulate laws and develop theories to better understand the behavior of the natural world. To do so, they operate in the macroscopic, microscopic, and symbolic domains. Chemists measure, analyze, purify, and synthesize a wide variety of substances that are important to our lives.

Glossary

chemistry
study of the composition, properties, and interactions of matter

hypothesis
tentative explanation of observations that acts as a guide for gathering and checking information

law
statement that summarizes a vast number of experimental observations, and describes or predicts some aspect of the natural world

macroscopic domain
realm of everyday things that are large enough to sense directly by human sight and touch

microscopic domain
realm of things that are much too small to be sensed directly

scientific method
path of discovery that leads from question and observation to law or hypothesis to theory, combined with experimental verification of the hypothesis and any necessary modification of the theory

symbolic domain
specialized language used to represent components of the macroscopic and microscopic domains, such as chemical symbols, chemical formulas, chemical equations, graphs, drawings, and calculations

theory
well-substantiated, comprehensive, testable explanation of a particular aspect of nature

---

This page titled 3: Ionic and Covalent Compounds is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.1: Chemistry in Context** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

3.1: Molecular and Ionic Compounds

Learning Objectives

By the end of this section, you will be able to:

- Define ionic and molecular (covalent) compounds
- Predict the type of compound formed from elements based on their location within the periodic table
- Determine formulas for simple ionic compounds

In ordinary chemical reactions, the nucleus of each atom (and thus the identity of the element) remains unchanged. Electrons, however, can be added to atoms by transfer from other atoms, lost by transfer to other atoms, or shared with other atoms. The transfer and sharing of electrons among atoms govern the chemistry of the elements. During the formation of some compounds, atoms gain or lose electrons, and form electrically charged particles called ions (Figure **3.1.1**).

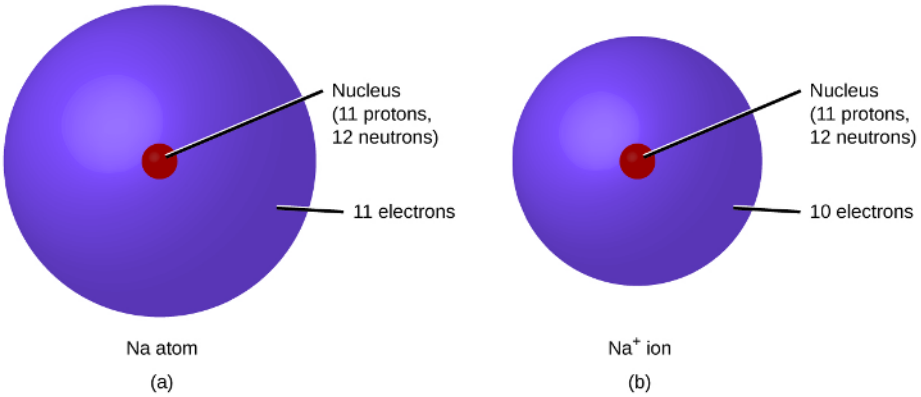


Table **3.1.1**: (a) A sodium atom (Na) has equal numbers of protons and electrons (11) and is uncharged. (b) A sodium cation (Na^+) has lost an electron, so it has one more proton (11) than electrons (10), giving it an overall positive charge, signified by a superscripted plus sign.

You can use the periodic table to predict whether an atom will form an anion or a cation, and you can often predict the charge of the resulting ion. Atoms of many main-group metals lose enough electrons to leave them with the same number of electrons as an atom of the preceding noble gas. To illustrate, an atom of an alkali metal (group 1) loses one electron and forms a cation with a 1+ charge; an alkaline earth metal (group 2) loses two electrons and forms a cation with a 2+ charge, and so on. For example, a neutral calcium atom, with 20 protons and 20 electrons, readily loses two electrons. This results in a cation with 20 protons, 18 electrons, and a 2+ charge. It has the same number of electrons as atoms of the preceding noble gas, argon, and is symbolized Ca^{2+}. The name of a metal ion is the same as the name of the metal atom from which it forms, so Ca^{2+} is called a calcium ion.

When atoms of nonmetal elements form ions, they generally gain enough electrons to give them the same number of electrons as an atom of the next noble gas in the periodic table. Atoms of group 17 gain one electron and form anions with a 1− charge; atoms of group 16 gain two electrons and form ions with a 2− charge, and so on. For example, the neutral bromine atom, with 35 protons and 35 electrons, can gain one electron to provide it with 36 electrons. This results in an anion with 35 protons, 36 electrons, and a 1− charge. It has the same number of electrons as atoms of the next noble gas, krypton, and is symbolized Br^-. (A discussion of the theory supporting the favored status of noble gas electron numbers reflected in these predictive rules for ion formation is provided in a later chapter of this text.)

Note the usefulness of the periodic table in predicting likely ion formation and charge (Figure **3.1.2**). Moving from the far left to the right on the periodic table, main-group elements tend to form cations with a charge equal to the group number. That is, group 1 elements form 1+ ions; group 2 elements form 2+ ions, and so on. Moving from the far right to the left on the periodic table, elements often form anions with a negative charge equal to the number of groups moved left from the noble gases. For example, group 17 elements (one group left of the noble gases) form 1− ions; group 16 elements (two groups left) form 2− ions, and so on. This trend can be used as a guide in many cases, but its predictive value decreases when moving toward the center of the periodic

table. In fact, transition metals and some other metals often exhibit variable charges that are not predictable by their location in the table. For example, copper can form ions with a 1+ or 2+ charge, and iron can form ions with a 2+ or 3+ charge.

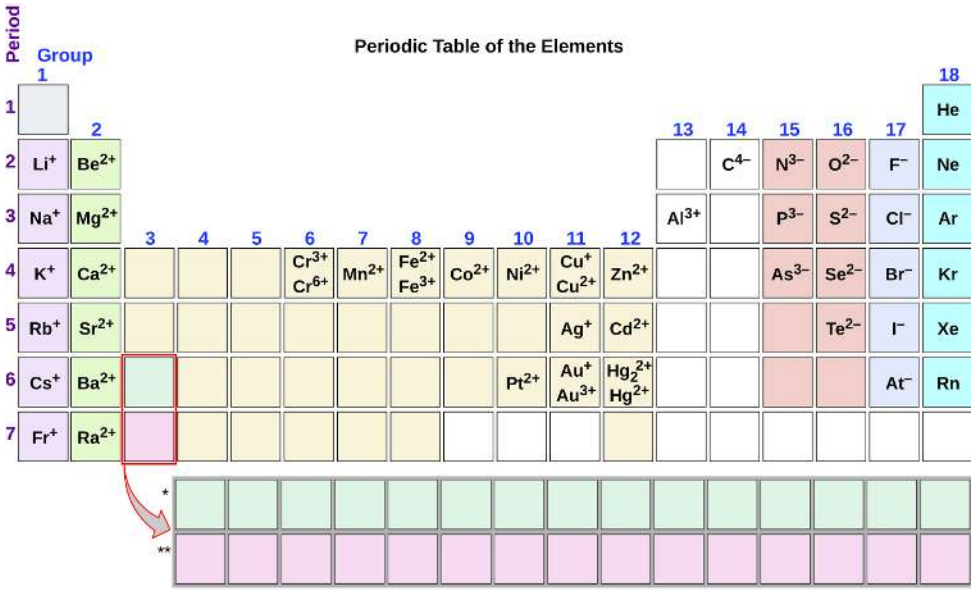


Table **3.1.2**: Some elements exhibit a regular pattern of ionic charge when they form ions.

✔ Example 3.1.1: Composition of Ions

An ion found in some compounds used as antiperspirants contains 13 protons and 10 electrons. What is its symbol?

Solution

Because the number of protons remains unchanged when an atom forms an ion, the atomic number of the element must be 13. Knowing this lets us use the periodic table to identify the element as Al (aluminum). The Al atom has lost three electrons and thus has three more positive charges (13) than it has electrons (10). This is the aluminum cation, Al^{3+}.

? Exercise 3.1.1

Give the symbol and name for the ion with 34 protons and 36 electrons.

Answer

Se^{2-}, the selenide ion

✔ Example 3.1.2: Formation of Ions

Magnesium and nitrogen react to form an ionic compound. Predict which forms an anion, which forms a cation, and the charges of each ion. Write the symbol for each ion and name them.

Solution

Magnesium's position in the periodic table (group 2) tells us that it is a metal. Metals form positive ions (cations). A magnesium atom must lose two electrons to have the same number electrons as an atom of the previous noble gas, neon. Thus, a magnesium atom will form a cation with two fewer electrons than protons and a charge of 2+. The symbol for the ion is Mg^{2+}, and it is called a magnesium ion.

Nitrogen's position in the periodic table (group 15) reveals that it is a nonmetal. Nonmetals form negative ions (anions). A nitrogen atom must gain three electrons to have the same number of electrons as an atom of the following noble gas, neon. Thus, a nitrogen atom will form an anion with three more electrons than protons and a charge of 3−. The symbol for the ion is N^{3-}, and it is called a nitride ion.

Exercise 3.1.2

Aluminum and carbon react to form an ionic compound. Predict which forms an anion, which forms a cation, and the charges of each ion. Write the symbol for each ion and name them.

Answer

Al will form a cation with a charge of 3+: Al^{3+}, an aluminum ion. Carbon will form an anion with a charge of 4−: C^{4-}, a carbide ion.

The ions that we have discussed so far are called monatomic ions, that is, they are ions formed from only one atom. We also find many polyatomic ions. These ions, which act as discrete units, are electrically charged molecules (a group of bonded atoms with an overall charge). Some of the more important polyatomic ions are listed in Table **3.1.1**. Oxyanions are polyatomic ions that contain one or more oxygen atoms. At this point in your study of chemistry, you should memorize the names, formulas, and charges of the most common polyatomic ions. Because you will use them repeatedly, they will soon become familiar.

Table **3.1.1**: Common Polyatomic Ions

Name	Formula	Related Acid	Formula
ammonium	NH_4^+		
hydronium	H_3O		
peroxide	O_2^{2-}		
hydroxide	OH^-		
acetate	CH_3COO^-	acetic acid	CH_3COOH
cyanide	CN^-	hydrocyanic acid	HCN
azide	N_3^-	hydrazoic acid	HN_3
carbonate	CO_3^{2-}	carbonic acid	H_2CO_3
bicarbonate	HCO_3^-		
nitrate	NO_3^-	nitric acid	HNO_3
nitrite	NO_2^-	nitrous acid	HNO_2
sulfate	SO_{42}^-	sulfuric acid	H_2SO_4
hydrogen sulfate	HSO_4^-		
sulfite	SO_3^{2-}	sulfurous acid	H_2SO_3
hydrogen sulfite	HSO_3^-		
phosphate	PO_4^{3-}	phosphoric acid	H_3PO_4
hydrogen phosphate	HPO_4^{2-}		
dihydrogen phosphate	$H_2PO_4^-$		
perchlorate	ClO_4^-	perchloric acid	$HClO_4$
chlorate	ClO_3^-	chloric acid	$HClO_3$
chlorite	ClO_2^-	chlorous acid	$HClO_2$
hypochlorite	ClO^-	hypochlorous acid	$HClO$
chromate	CrO_4^{2-}	chromic acid	H_2CrO_4
dichromate	$Cr_2O_7^{2-}$	dichromic acid	$H_2Cr_2O_7$
permanganate	MnO_4^-	permanganic acid	$HMnO_4$

Note that there is a system for naming some polyatomic ions; -ate and -ite are suffixes designating polyatomic ions containing more or fewer oxygen atoms. Per- (short for “hyper”) and hypo- (meaning “under”) are prefixes meaning more oxygen atoms than -ate and fewer oxygen atoms than -ite, respectively. For example, perchlorate is ClO_4^-, chlorate is ClO_3^-, chlorite is ClO_2^- and hypochlorite is ClO^-. Unfortunately, the number of oxygen atoms corresponding to a given suffix or prefix is not consistent; for example, nitrate is NO_3^- while sulfate is SO_4^{2-}. This will be covered in more detail in the next module on nomenclature.

The nature of the attractive forces that hold atoms or ions together within a compound is the basis for classifying chemical bonding. When electrons are transferred and ions form, ionic bonds result. Ionic bonds are electrostatic forces of attraction, that is, the attractive forces experienced between objects of opposite electrical charge (in this case, cations and anions). When electrons are “shared” and molecules form, covalent bonds result. Covalent bonds are the attractive forces between the positively charged nuclei

of the bonded atoms and one or more pairs of electrons that are located between the atoms. Compounds are classified as ionic or molecular (covalent) on the basis of the bonds present in them.

3.1.1: Ionic Compounds

When an element composed of atoms that readily lose electrons (a metal) reacts with an element composed of atoms that readily gain electrons (a nonmetal), a transfer of electrons usually occurs, producing ions. The compound formed by this transfer is stabilized by the electrostatic attractions (ionic bonds) between the ions of opposite charge present in the compound. For example, when each sodium atom in a sample of sodium metal (group 1) gives up one electron to form a sodium cation, Na^+, and each chlorine atom in a sample of chlorine gas (group 17) accepts one electron to form a chloride anion, Cl^-, the resulting compound, NaCl, is composed of sodium ions and chloride ions in the ratio of one Na^+ ion for each Cl^- ion. Similarly, each calcium atom (group 2) can give up two electrons and transfer one to each of two chlorine atoms to form $CaCl_2$, which is composed of Ca^{2+} and Cl^- ions in the ratio of one Ca^{2+} ion to two Cl^- ions.

A compound that contains ions and is held together by ionic bonds is called an ionic compound. The periodic table can help us recognize many of the compounds that are ionic: When a metal is combined with one or more nonmetals, the compound is usually ionic. This guideline works well for predicting ionic compound formation for most of the compounds typically encountered in an introductory chemistry course. However, it is not always true (for example, aluminum chloride, $AlCl_3$, is not ionic).

You can often recognize ionic compounds because of their properties. Ionic compounds are solids that typically melt at high temperatures and boil at even higher temperatures. For example, sodium chloride melts at 801 °C and boils at 1413 °C. (As a comparison, the molecular compound water melts at 0 °C and boils at 100 °C.) In solid form, an ionic compound is not electrically conductive because its ions are unable to flow (“electricity” is the flow of charged particles). When molten, however, it can conduct electricity because its ions are able to move freely through the liquid (Figure **3.1.3**).

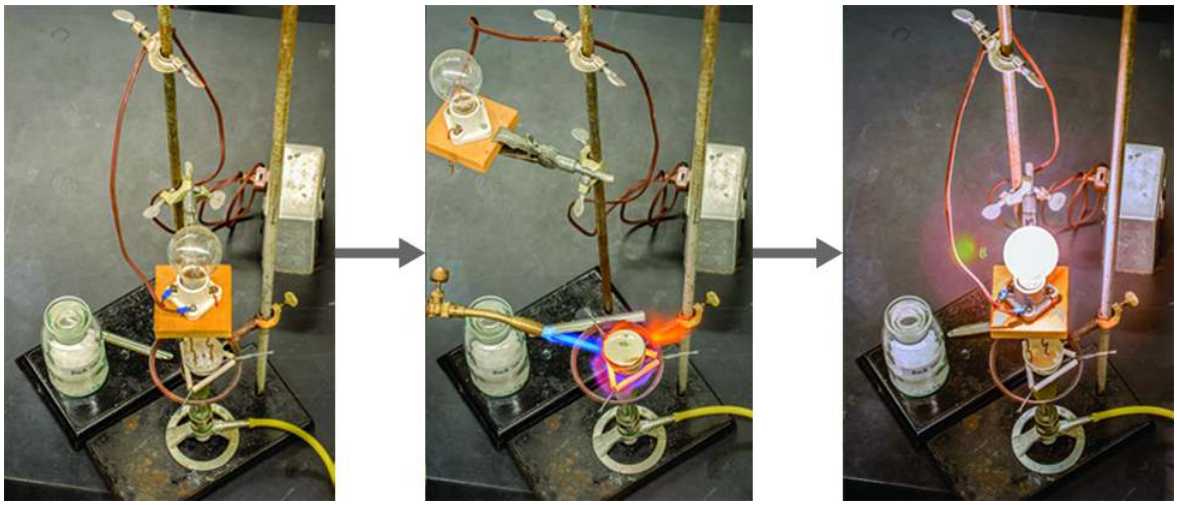


Table **3.1.3**: Sodium chloride melts at 801 °C and conducts electricity when molten. (credit: modification of work by Mark Blaser and Matt Evans)

Link to Learning

Watch this video to see a mixture of salts melt and conduct electricity.

In every ionic compound, the total number of positive charges of the cations equals the total number of negative charges of the anions. Thus, ionic compounds are electrically neutral overall, even though they contain positive and negative ions. We can use this observation to help us write the formula of an ionic compound. The formula of an ionic compound must have a ratio of ions such that the numbers of positive and negative charges are equal.

Example 3.1.3: Predicting the Formula of an Ionic Compound

The gemstone sapphire (Figure **3.1.4**) is mostly a compound of aluminum and oxygen that contains aluminum cations, Al^{3+}, and oxygen anions, O^{2-}. What is the formula of this compound?



Table **3.1.4**: Although pure aluminum oxide is colorless, trace amounts of iron and titanium give blue sapphire its characteristic color. (credit: modification of work by Stanislav Doronenko via Wikipedia)

Solution

Because the ionic compound must be electrically neutral, it must have the same number of positive and negative charges. Two aluminum ions, each with a charge of 3+, would give us six positive charges, and three oxide ions, each with a charge of 2−, would give us six negative charges. The formula would be Al_2O_3.

Exercise 3.1.3

Predict the formula of the ionic compound formed between the sodium cation, Na^+, and the sulfide anion, S^{2-}.

Answer

Na_2S

Many ionic compounds contain polyatomic ions (Table **3.1.1**) as the cation, the anion, or both. As with simple ionic compounds, these compounds must also be electrically neutral, so their formulas can be predicted by treating the polyatomic ions as discrete units. We use parentheses in a formula to indicate a group of atoms that behave as a unit. For example, the formula for calcium phosphate, one of the minerals in our bones, is $\mathbf{Ca_3(PO_4)_2}$. This formula indicates that there are three calcium ions ($\mathbf{Ca^{2+}}$) for every two phosphate ($\mathbf{PO_4^{3-}}$) groups. The $\mathbf{PO_4^{3-}}$ groups are discrete units, each consisting of one phosphorus atom and four oxygen atoms, and having an overall charge of 3−. The compound is electrically neutral, and its formula shows a total count of three Ca, two P, and eight O atoms.

Example 3.1.4: Predicting the Formula of a Compound with a Polyatomic Anion

Baking powder contains calcium dihydrogen phosphate, an ionic compound composed of the ions $\mathbf{Ca^{2+}}$ and $\mathbf{H_2PO_4^-}$. What is the formula of this compound?

Solution

The positive and negative charges must balance, and this ionic compound must be electrically neutral. Thus, we must have two negative charges to balance the 2+ charge of the calcium ion. This requires a ratio of one Ca^{2+} ion to two $\mathbf{H_2PO_4^-}$ ions. We designate this by enclosing the formula for the dihydrogen phosphate ion in parentheses and adding a subscript 2. The formula is $Ca(H_2PO_4)_2$.

Exercise 3.1.4

Predict the formula of the ionic compound formed between the lithium ion and the peroxide ion, $\mathbf{O_2^{2-}}$ (Hint: Use the periodic table to predict the sign and the charge on the lithium ion.)

Answer

Li_2O_2

Because an ionic compound is not made up of single, discrete molecules, it may not be properly symbolized using a *molecular* formula. Instead, ionic compounds must be symbolized by a formula indicating the relative numbers of its constituent ions. For compounds containing only monatomic ions (such as $NaCl$) and for many compounds containing polyatomic ions (such as $CaSO_4$), these formulas are just the empirical formulas introduced earlier in this chapter. However, the formulas for some ionic compounds containing polyatomic ions are not empirical formulas. For example, the ionic compound sodium oxalate is comprised of Na^+ and $C_2O_4^{2-}$ ions combined in a 2:1 ratio, and its formula is written as $Na_2C_2O_4$. The subscripts in this formula are not the smallest-possible whole numbers, as each can be divided by 2 to yield the empirical formula, $NaCO_2$. This is not the accepted formula for sodium oxalate, however, as it does not accurately represent the compound's polyatomic anion, $C_2O_4^{2-}$.

3.1.2: Molecular Compounds

Many compounds do not contain ions but instead consist solely of discrete, neutral molecules. These molecular compounds (covalent compounds) result when atoms share, rather than transfer (gain or lose), electrons. Covalent bonding is an important and extensive concept in chemistry, and it will be treated in considerable detail in a later chapter of this text. We can often identify molecular compounds on the basis of their physical properties. Under normal conditions, molecular compounds often exist as gases, low-boiling liquids, and low-melting solids, although many important exceptions exist.

Whereas ionic compounds are usually formed when a metal and a nonmetal combine, covalent compounds are usually formed by a combination of nonmetals. Thus, the periodic table can help us recognize many of the compounds that are covalent. While we can use the positions of a compound's elements in the periodic table to predict whether it is ionic or covalent at this point in our study of chemistry, you should be aware that this is a very simplistic approach that does not account for a number of interesting exceptions. Shades of gray exist between ionic and molecular compounds, and you'll learn more about those later.

✔ Example 3.1.5: Predicting the Type of Bonding in Compounds

Predict whether the following compounds are ionic or molecular:

a. KI, the compound used as a source of iodine in table salt
b. H_2O_2, the bleach and disinfectant hydrogen peroxide
c. $CHCl_3$, the anesthetic chloroform
d. Li_2CO_3, a source of lithium in antidepressants

Solution

a. Potassium (group 1) is a metal, and iodine (group 17) is a nonmetal; KI is predicted to be ionic.
b. Hydrogen (group 1) is a nonmetal, and oxygen (group 16) is a nonmetal; H_2O_2 is predicted to be molecular.
c. Carbon (group 14) is a nonmetal, hydrogen (group 1) is a nonmetal, and chlorine (group 17) is a nonmetal; $CHCl_3$ is predicted to be molecular.
d. Lithium (group 1) is a metal, and carbonate is a polyatomic ion; Li_2CO_3 is predicted to be ionic.

? Exercise 3.1.5

Using the periodic table, predict whether the following compounds are ionic or covalent:

a. SO_2
b. CaF_2
c. N_2H_4
d. $Al_2(SO_4)_3$

Answer

a. molecular
b. ionic

c. molecular
d. ionic

This page titled 3.1: Molecular and Ionic Compounds is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **2.6: Molecular and Ionic Compounds** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

3.2: Ionic Bonding

Learning Objectives

By the end of this section, you will be able to:

- Explain the formation of cations, anions, and ionic compounds
- Predict the charge of common metallic and nonmetallic elements, and write their electron configurations

As you have learned, ions are atoms or molecules bearing an electrical charge. A cation (a positive ion) forms when a neutral atom loses one or more electrons from its valence shell, and an anion (a negative ion) forms when a neutral atom gains one or more electrons in its valence shell.

Compounds composed of ions are called ionic compounds (or salts), and their constituent ions are held together by ionic bonds: electrostatic forces of attraction between oppositely charged cations and anions. The properties of ionic compounds shed some light on the nature of ionic bonds. Ionic solids exhibit a crystalline structure and tend to be rigid and brittle; they also tend to have high melting and boiling points, which suggests that ionic bonds are very strong. Ionic solids are also poor conductors of electricity for the same reason—the strength of ionic bonds prevents ions from moving freely in the solid state. Most ionic solids, however, dissolve readily in water. Once dissolved or melted, ionic compounds are excellent conductors of electricity and heat because the ions can move about freely.

Neutral atoms and their associated ions have very different physical and chemical properties. Sodium *atoms* form sodium metal, a soft, silvery-white metal that burns vigorously in air and reacts explosively with water. Chlorine *atoms* form chlorine gas, Cl_2, a yellow-green gas that is extremely corrosive to most metals and very poisonous to animals and plants. The vigorous reaction between the elements sodium and chlorine forms the white, crystalline compound sodium chloride, common table salt, which contains sodium *cations* and chloride *anions* (Figure **3.2.1**). The compound composed of these ions exhibits properties entirely different from the properties of the elements sodium and chlorine. Chlorine is poisonous, but sodium chloride is essential to life; sodium atoms react vigorously with water, but sodium chloride simply dissolves in water.



Figure **3.2.1**: (a) Sodium is a soft metal that must be stored in mineral oil to prevent reaction with air or water. (b) Chlorine is a pale yellow-green gas. (c) When combined, they form white crystals of sodium chloride (table salt). (credit a: modification of work by "Jurii"/Wikimedia Commons)

3.2.1: The Formation of Ionic Compounds

Binary ionic compounds are composed of just two elements: a metal (which forms the cations) and a nonmetal (which forms the anions). For example, NaCl is a binary ionic compound. We can think about the formation of such compounds in terms of the periodic properties of the elements. Many metallic elements have relatively low ionization potentials and lose electrons easily. These elements lie to the left in a period or near the bottom of a group on the periodic table. Nonmetal atoms have relatively high electron affinities and thus readily gain electrons lost by metal atoms, thereby filling their valence shells. Nonmetallic elements are found in the upper-right corner of the periodic table.

As all substances must be electrically neutral, the total number of positive charges on the cations of an ionic compound must equal the total number of negative charges on its anions. The formula of an ionic compound represents the simplest ratio of the numbers of ions necessary to give identical numbers of positive and negative charges. For example, the formula for aluminum oxide, Al_2O_3,

indicates that this ionic compound contains two aluminum cations, Al^{3+}, for every three oxide anions, O^{2-} [thus, (2 +3) + (3 –2) = 0].

It is important to note, however, that the formula for an ionic compound does *not* represent the physical arrangement of its ions. It is incorrect to refer to a sodium chloride (NaCl) "molecule" because there is not a single ionic bond, per se, between any specific pair of sodium and chloride ions. The attractive forces between ions are isotropic—the same in all directions—meaning that any particular ion is equally attracted to all of the nearby ions of opposite charge. This results in the ions arranging themselves into a tightly bound, three-dimensional lattice structure. Sodium chloride, for example, consists of a regular arrangement of equal numbers of Na^+ cations and Cl^- anions (Figure **3.2.2**).

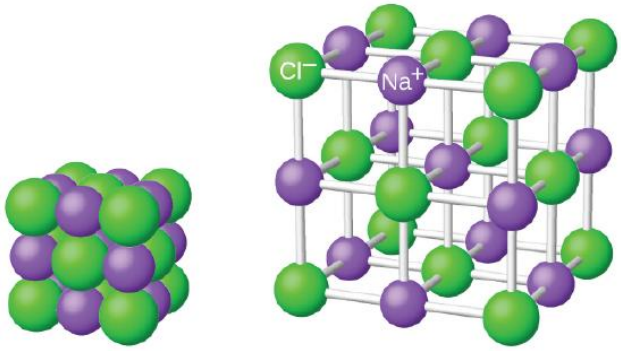


Figure **3.2.2**: The atoms in sodium chloride (common table salt) are arranged to (a) maximize opposite charges interacting. The smaller spheres represent sodium ions, the larger ones represent chloride ions. In the expanded view (b), the geometry can be seen more clearly. Note that each ion is "bonded" to all of the surrounding ions—six in this case.

The strong electrostatic attraction between Na^+ and Cl^- ions holds them tightly together in solid NaCl. It requires 769 kJ of energy to dissociate one mole of solid NaCl into separate gaseous Na^+ and Cl^- ions:

$$\mathrm{NaCl\,(s) \longrightarrow Na^+\,(g) + Cl^-\,(g)} \qquad \Delta H = 769\,\mathrm{kJ}$$

3.2.2: Electronic Structures of Cations

When forming a cation, an atom of a main group element tends to lose all of its valence electrons, thus assuming the electronic structure of the noble gas that precedes it in the periodic table. For groups 1 (the alkali metals) and 2 (the alkaline earth metals), the group numbers are equal to the numbers of valence shell electrons and, consequently, to the charges of the cations formed from atoms of these elements when all valence shell electrons are removed. For example, calcium is a group 2 element whose neutral atoms have 20 electrons and a ground state electron configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$. When a Ca atom loses both of its valence electrons, the result is a cation with 18 electrons, a 2+ charge, and an electron configuration of $1s^2 2s^2 2p^6 3s^2 3p^6$. The Ca^{2+} ion is therefore isoelectronic with the noble gas Ar.

For groups 13–17, the group numbers exceed the number of valence electrons by 10 (accounting for the possibility of full *d* subshells in atoms of elements in the fourth and greater periods). Thus, the charge of a cation formed by the loss of all valence electrons is equal to the group number minus 10. For example, aluminum (in group 13) forms 3+ ions (Al^{3+}).

Exceptions to the expected behavior involve elements toward the bottom of the groups. In addition to the expected ions Tl^{3+}, Sn^{4+}, Pb^{4+}, and Bi^{5+}, a partial loss of these atoms' valence shell electrons can also lead to the formation of Tl^+, Sn^{2+}, Pb^{2+}, and Bi^{3+} ions. The formation of these 1+, 2+, and 3+ cations is ascribed to the inert pair effect, which reflects the relatively low energy of the valence *s*-electron pair for atoms of the heavy elements of groups 13, 14, and 15. Mercury (group 12) also exhibits an unexpected behavior: it forms a diatomic ion, (an ion formed from two mercury atoms, with an Hg-Hg bond), in addition to the expected monatomic ion Hg^{2+} (formed from only one mercury atom).

Transition and inner transition metal elements behave differently than main group elements. Most transition metal cations have 2+ or 3+ charges that result from the loss of their outermost *s* electron(s) first, sometimes followed by the loss of one or two *d* electrons from the next-to-outermost shell. For example, iron ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$) forms the ion Fe^{2+} ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$) by the loss of the 4*s* electrons and the ion Fe^{3+} ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$) by the loss of the 4*s* electrons and one of the 3*d* electrons.

Although the *d* orbitals of the transition elements are—according to the Aufbau principle—the last to fill when building up electron configurations, the outermost *s* electrons are the first to be lost when these atoms ionize. When the inner transition metals form ions, they usually have a 3+ charge, resulting from the loss of their outermost *s* electrons and a *d* or *f* electron.

Example 3.2.1: Determining the Electronic Structures of Cations

There are at least 14 elements categorized as "essential trace elements" for the human body. They are called "essential" because they are required for healthy bodily functions, "trace" because they are required only in small amounts, and "elements" in spite of the fact that they are really ions. Two of these essential trace elements, chromium and zinc, are required as Cr^{3+} and Zn^{2+}. Write the electron configurations of these cations.

Solution

First, write the electron configuration for the neutral atoms:

Zn: $[Ar]3d^{10}4s^2$

Cr: $[Ar]3d^5 4s^1$

Next, remove electrons from the highest energy orbital. For the transition metals, electrons are removed from the *s* orbital first and then from the *d* orbital. For the *p*-block elements, electrons are removed from the *p* orbitals and then from the *s* orbital. Zinc is a member of group 12, so it should have a charge of 2+, and thus loses only the two electrons in its *s* orbital. Chromium is a transition element and should lose its *s* electrons and then its *d* electrons when forming a cation. Thus, we find the following electron configurations of the ions:

Zn^{2+}: $[Ar]3d^{10}$

Cr^{3+}: $[Ar]3d^3$

Exercise 3.2.1

Potassium and magnesium are required in our diet. Write the electron configurations of the ions expected from these elements.

Answer

K^+: [Ar], Mg^{2+}: [Ne]

3.2.3: Electronic Structures of Anions

Most monatomic anions form when a neutral nonmetal atom gains enough electrons to completely fill its outer *s* and *p* orbitals, thereby reaching the electron configuration of the next noble gas. Thus, it is simple to determine the charge on such a negative ion: The charge is equal to the number of electrons that must be gained to fill the *s* and *p* orbitals of the parent atom. Oxygen, for example, has the electron configuration $1s^2 2s^2 2p^4$, whereas the oxygen anion has the electron configuration of the noble gas neon (Ne), $1s^2 2s^2 2p^6$. The two additional electrons required to fill the valence orbitals give the oxide ion the charge of 2– (O^{2-}).

Example 3.2.1: Determining the Electronic Structure of Anions

Selenium and iodine are two essential trace elements that form anions. Write the electron configurations of the anions.

Solution

Se^{2-}: $[Ar]3d^{10}4s^2 4p^6$

I^-: $[Kr]4d^{10}5s^2 5p^6$

Exercise 3.2.2

Write the electron configurations of a phosphorus atom and its negative ion. Give the charge on the anion.

Answer

P: [Ne]$3s^2 3p^3$; P^{3-}: [Ne]$3s^2 3p^6$

This page titled 3.2: Ionic Bonding is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **7.1: Ionic Bonding** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

3.3: Covalent Bonding

Learning Objectives

By the end of this section, you will be able to:

- Describe the formation of covalent bonds
- Define electronegativity and assess the polarity of covalent bonds

Ionic bonding results from the electrostatic attraction of oppositely charged ions that are typically produced by the transfer of electrons between metallic and nonmetallic atoms. A different type of bonding results from the mutual attraction of atoms for a "shared" pair of electrons. Such bonds are called covalent bonds. Covalent bonds are formed between two atoms when both have similar tendencies to attract electrons to themselves (i.e., when both atoms have identical or fairly similar ionization energies and electron affinities). For example, two hydrogen atoms bond covalently to form an H_2 molecule; each hydrogen atom in the H_2 molecule has two electrons stabilizing it, giving each atom the same number of valence electrons as the noble gas He.

Compounds that contain covalent bonds exhibit different physical properties than ionic compounds. Because the attraction between molecules, which are electrically neutral, is weaker than that between electrically charged ions, covalent compounds generally have much lower melting and boiling points than ionic compounds. In fact, many covalent compounds are liquids or gases at room temperature, and, in their solid states, they are typically much softer than ionic solids. Furthermore, whereas ionic compounds are good conductors of electricity when dissolved in water, most covalent compounds are insoluble in water; since they are electrically neutral, they are poor conductors of electricity in any state.

3.3.1: Formation of Covalent Bonds

Nonmetal atoms frequently form covalent bonds with other nonmetal atoms. For example, the hydrogen molecule, H_2, contains a covalent bond between its two hydrogen atoms. Figure **3.3.1** illustrates why this bond is formed. Starting on the far right, we have two separate hydrogen atoms with a particular potential energy, indicated by the red line. Along the *x*-axis is the distance between the two atoms. As the two atoms approach each other (moving left along the *x*-axis), their valence orbitals (1*s*) begin to overlap. The single electrons on each hydrogen atom then interact with both atomic nuclei, occupying the space around both atoms. The strong attraction of each shared electron to both nuclei stabilizes the system, and the potential energy decreases as the bond distance decreases. If the atoms continue to approach each other, the positive charges in the two nuclei begin to repel each other, and the potential energy increases. The bond length is determined by the distance at which the lowest potential energy is achieved.

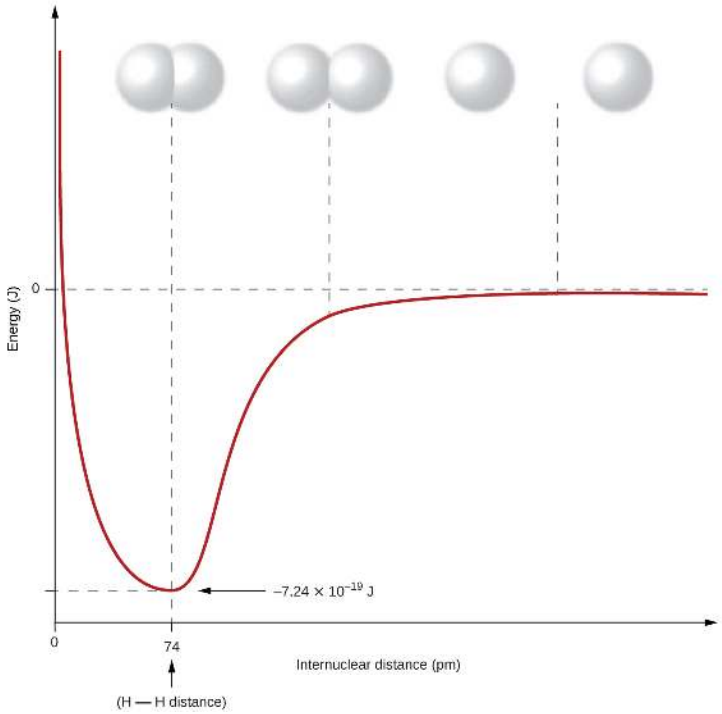


Figure **3.3.1**: The potential energy of two separate hydrogen atoms (right) decreases as they approach each other, and the single electrons on each atom are shared to form a covalent bond. The bond length is the internuclear distance at which the lowest potential energy is achieved.

It is essential to remember that energy must be added to break chemical bonds (an endothermic process), whereas forming chemical bonds releases energy (an exothermic process). In the case of H_2, the covalent bond is very strong; a large amount of energy, 436 kJ, must be added to break the bonds in one mole of hydrogen molecules and cause the atoms to separate:

$$\mathrm{H_2\,(g) \longrightarrow 2\,H\,(g)} \quad \Delta H = 436\,\mathrm{kJ}$$

Conversely, the same amount of energy is released when one mole of H_2 molecules forms from two moles of H atoms:

$$\mathrm{2\,H\,(g) \longrightarrow H_2\,(g)} \quad \Delta H = -436\,\mathrm{kJ}$$

3.3.2: Pure vs. Polar Covalent Bonds

If the atoms that form a covalent bond are identical, as in H_2, Cl_2, and other diatomic molecules, then the electrons in the bond must be shared equally. We refer to this as a pure covalent bond. Electrons shared in pure covalent bonds have an equal probability of being near each nucleus.

In the case of Cl_2, each atom starts off with seven valence electrons, and each Cl shares one electron with the other, forming one covalent bond:

$$\mathrm{Cl + Cl \longrightarrow Cl_2}$$

The total number of electrons around each individual atom consists of six nonbonding electrons and two shared (i.e., bonding) electrons for eight total electrons, matching the number of valence electrons in the noble gas argon. Since the bonding atoms are identical, Cl_2 also features a pure covalent bond.

When the atoms linked by a covalent bond are different, the bonding electrons are shared, but no longer equally. Instead, the bonding electrons are more attracted to one atom than the other, giving rise to a shift of electron density toward that atom. This unequal distribution of electrons is known as a polar covalent bond, characterized by a partial positive charge on one atom and a partial negative charge on the other. The atom that attracts the electrons more strongly acquires the partial negative charge and vice versa. For example, the electrons in the H–Cl bond of a hydrogen chloride molecule spend more time near the chlorine atom than near the hydrogen atom. Thus, in an HCl molecule, the chlorine atom carries a partial negative charge and the hydrogen atom has a partial positive charge. Figure **3.3.2** shows the distribution of electrons in the H–Cl bond. Note that the shaded area around Cl is

much larger than it is around H. Compare this to Figure **3.3.1**, which shows the even distribution of electrons in the H_2 nonpolar bond.

We sometimes designate the positive and negative atoms in a polar covalent bond using a lowercase Greek letter "delta," δ, with a plus sign or minus sign to indicate whether the atom has a partial positive charge (δ+) or a partial negative charge (δ–). This symbolism is shown for the H–Cl molecule in Figure **3.3.2**.

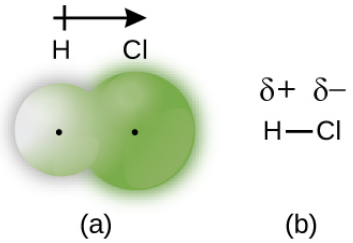


Figure **3.3.2**: (a) The distribution of electron density in the HCl molecule is uneven. The electron density is greater around the chlorine nucleus. The small, black dots indicate the location of the hydrogen and chlorine nuclei in the molecule. (b) Symbols δ+ and δ– indicate the polarity of the H–Cl bond.

3.3.3: Electronegativity

Whether a bond is nonpolar or polar covalent is determined by a property of the bonding atoms called electronegativity. Electronegativity is a measure of the tendency of an atom to attract electrons (or electron density) towards itself. It determines how the shared electrons are distributed between the two atoms in a bond. The more strongly an atom attracts the electrons in its bonds, the larger its electronegativity. Electrons in a polar covalent bond are shifted toward the more electronegative atom; thus, the more electronegative atom is the one with the partial negative charge. The greater the difference in electronegativity, the more polarized the electron distribution and the larger the partial charges of the atoms.

Figure **3.3.3** shows the electronegativity values of the elements as proposed by one of the most famous chemists of the twentieth century: Linus Pauling (Figure **3.3.4**). In general, electronegativity increases from left to right across a period in the periodic table and decreases down a group. Thus, the nonmetals, which lie in the upper right, tend to have the highest electronegativities, with fluorine the most electronegative element of all (EN = 4.0). Metals tend to be less electronegative elements, and the group 1 metals have the lowest electronegativities. Note that noble gases are excluded from this figure because these atoms usually do not share electrons with others atoms since they have a full valence shell. (While noble gas compounds such as XeO_2 do exist, they can only be formed under extreme conditions, and thus they do not fit neatly into the general model of electronegativity.)

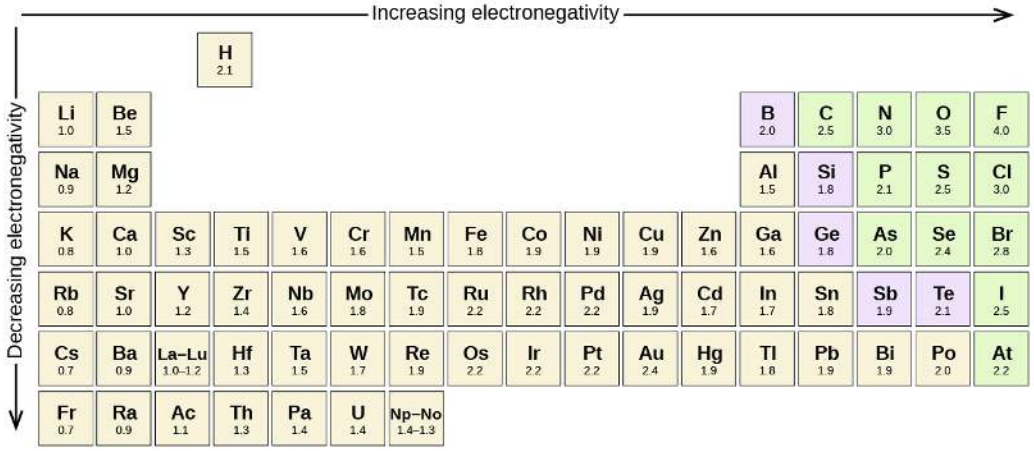


Figure **3.3.3**: The electronegativity values derived by Pauling follow predictable periodic trends, with the higher electronegativities toward the upper right of the periodic table.

3.3.3.1: Electronegativity versus Electron Affinity

We must be careful not to confuse electronegativity and electron affinity. The electron affinity of an element is a measurable physical quantity, namely, the energy released or absorbed when an isolated gas-phase atom acquires an electron, measured in kJ/mol. Electronegativity, on the other hand, describes how tightly an atom attracts electrons in a bond. It is a dimensionless

quantity that is calculated, not measured. Pauling derived the first electronegativity values by comparing the amounts of energy required to break different types of bonds. He chose an arbitrary relative scale ranging from 0 to 4.

Portrait of a Chemist: Linus Pauling

Linus Pauling, shown in Figure **3.3.4**, is the only person to have received two unshared (individual) Nobel Prizes: one for chemistry in 1954 for his work on the nature of chemical bonds and one for peace in 1962 for his opposition to weapons of mass destruction. He developed many of the theories and concepts that are foundational to our current understanding of chemistry, including electronegativity and resonance structures.

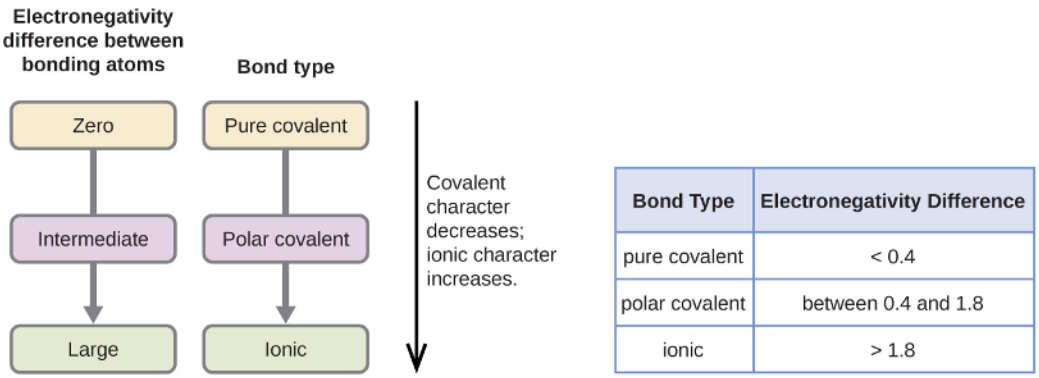


Figure **3.3.4**: Linus Pauling (1901–1994) made many important contributions to the field of chemistry. He was also a prominent activist, publicizing issues related to health and nuclear weapons.

Pauling also contributed to many other fields besides chemistry. His research on sickle cell anemia revealed the cause of the disease—the presence of a genetically inherited abnormal protein in the blood—and paved the way for the field of molecular genetics. His work was also pivotal in curbing the testing of nuclear weapons; he proved that radioactive fallout from nuclear testing posed a public health risk.

3.3.3.2: Electronegativity and Bond Type

The absolute value of the difference in electronegativity (ΔEN) of two bonded atoms provides a rough measure of the polarity to be expected in the bond and, thus, the bond type. When the difference is very small or zero, the bond is covalent and nonpolar. When it is large, the bond is polar covalent or ionic. The absolute values of the electronegativity differences between the atoms in the bonds H–H, H–Cl, and Na–Cl are 0 (nonpolar), 0.9 (polar covalent), and 2.1 (ionic), respectively. The degree to which electrons are shared between atoms varies from completely equal (pure covalent bonding) to not at all (ionic bonding). Figure **3.3.5** shows the relationship between electronegativity difference and bond type.



Bond Type	Electronegativity Difference
pure covalent	< 0.4
polar covalent	between 0.4 and 1.8
ionic	> 1.8

Figure **3.3.5**: As the electronegativity difference increases between two atoms, the bond becomes more ionic.

A rough approximation of the electronegativity differences associated with covalent, polar covalent, and ionic bonds is shown in Figure **3.3.5**. This table is just a general guide, however, with many exceptions. For example, the H and F atoms in HF have an electronegativity difference of 1.9, and the N and H atoms in NH_3 a difference of 0.9, yet both of these compounds form bonds that

are considered polar covalent. Likewise, the Na and Cl atoms in NaCl have an electronegativity difference of 2.1, and the Mn and I atoms in MnI_2 have a difference of 1.0, yet both of these substances form ionic compounds.

The best guide to the covalent or ionic character of a bond is to consider the types of atoms involved and their relative positions in the periodic table. Bonds between two nonmetals are generally covalent; bonding between a metal and a nonmetal is often ionic.

Some compounds contain both covalent and ionic bonds. The atoms in polyatomic ions, such as OH^-, and are held together by polar covalent bonds. However, these polyatomic ions form ionic compounds by combining with ions of opposite charge. For example, potassium nitrate, KNO_3, contains the K^+ cation and the polyatomic anion. Thus, bonding in potassium nitrate is ionic, resulting from the electrostatic attraction between the ions K^+ and as well as covalent between the nitrogen and oxygen atoms in

Example 3.3.1: Electronegativity and Bond Polarity

Bond polarities play an important role in determining the structure of proteins. Using the electronegativity values in Figure **3.3.3**, arrange the following covalent bonds—all commonly found in amino acids—in order of increasing polarity. Then designate the positive and negative atoms using the symbols δ+ and δ–:

C–H, C–N, C–O, N–H, O–H, S–H

Solution

The polarity of these bonds increases as the absolute value of the electronegativity difference increases. The atom with the δ– designation is the more electronegative of the two. Table **3.3.1** shows these bonds in order of increasing polarity.

Table **3.3.1**: Bond Polarity and Electronegativity Difference

Bond	ΔEN	Polarity
C–H	0.4	
S–H	0.4	
C–N	0.5	
N–H	0.9	
C–O	1.0	
O–H	1.4	

Exercise 3.3.1

Silicones are polymeric compounds containing, among others, the following types of covalent bonds: Si–O, Si–C, C–H, and C–C. Using the electronegativity values in Figure **3.3.3**, arrange the bonds in order of increasing polarity and designate the positive and negative atoms using the symbols δ+ and δ–.

Answer

Bond	Electronegativity Difference	Polarity
C–C	0.0	nonpolar
C–H	0.4	
Si–C	0.7	
Si–O	1.7	

This page titled 3.3: Covalent Bonding is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **7.2: Covalent Bonding** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

3.4: Chemical Nomenclature

Learning Objectives

By the end of this section, you will be able to:

- Derive names for common types of inorganic compounds using a systematic approach

Nomenclature, a collection of rules for naming things, is important in science and in many other situations. This module describes an approach that is used to name simple ionic and molecular compounds, such as NaCl, $CaCO_3$, and N_2O_4. The simplest of these are **binary compounds**, those containing only two elements, but we will also consider how to name ionic compounds containing polyatomic ions, and one specific, very important class of compounds known as acids (subsequent chapters in this text will focus on these compounds in great detail). We will limit our attention here to inorganic compounds, compounds that are composed principally of elements other than carbon, and will follow the nomenclature guidelines proposed by IUPAC. The rules for organic compounds, in which carbon is the principle element, will be treated in a later chapter on organic chemistry.

3.4.1: Ionic Compounds

To name an inorganic compound, we need to consider the answers to several questions. First, is the compound ionic or molecular? If the compound is ionic, does the metal form ions of only one type (fixed charge) or more than one type (variable charge)? Are the ions monatomic or polyatomic? If the compound is molecular, does it contain hydrogen? If so, does it also contain oxygen? From the answers we derive, we place the compound in an appropriate category and then name it accordingly.

3.4.2: Compounds Containing Only Monatomic Ions

The name of a binary compound containing monatomic ions consists of the name of the cation (the name of the metal) followed by the name of the anion (the name of the nonmetallic element with its ending replaced by the suffix *–ide*). Some examples are given in Table **3.4.1**.

Table **3.4.1**: Names of Some Ionic Compounds

NaCl, sodium chloride	Na_2O, sodium oxide
KBr, potassium bromide	CdS, cadmium sulfide
CaI_2, calcium iodide	Mg_3N_2, magnesium nitride
CsF, cesium fluoride	Ca_3P_2, calcium phosphide
LiCl, lithium chloride	Al_4C_3, aluminum carbide

3.4.3: Compounds Containing Polyatomic Ions

Compounds containing polyatomic ions are named similarly to those containing only monatomic ions, i.e. by naming first the cation and then the anion. Examples are shown in Table **3.4.2**.

Table **3.4.2**: Names of Some Polyatomic Ionic Compounds

$KC_2H_3O_2$, potassium acetate	NH_4Cl, ammonium chloride
$NaHCO_3$, sodium bicarbonate	$CaSO_4$, calcium sulfate
$Al_2(CO_3)_3$, aluminum carbonate	$Mg_3(PO_4)_2$, magnesium phosphate

Chemistry in Everyday Life: Ionic Compounds in Your Cabinet

Every day you encounter and use a large number of ionic compounds. Some of these compounds, where they are found, and what they are used for are listed in Table **3.4.3**. Look at the label or ingredients list on the various products that you use during

the next few days, and see if you run into any of those in this table, or find other ionic compounds that you could now name or write as a formula.

Table **3.4.3**: Everyday Ionic Compounds

Ionic Compound	Use
NaCl, sodium chloride	ordinary table salt
KI, potassium iodide	added to “iodized” salt for thyroid health
NaF, sodium fluoride	ingredient in toothpaste
$NaHCO_3$, sodium bicarbonate	baking soda; used in cooking (and as antacid)
Na_2CO_3, sodium carbonate	washing soda; used in cleaning agents
NaOCl, sodium hypochlorite	active ingredient in household bleach
$CaCO_3$ calcium carbonate	ingredient in antacids
$Mg(OH)_2$, magnesium hydroxide	ingredient in antacids
$Al(OH)_3$, aluminum hydroxide	ingredient in antacids
NaOH, sodium hydroxide	lye; used as drain cleaner
K_3PO_4, potassium phosphate	food additive (many purposes)
$MgSO_4$, magnesium sulfate	added to purified water
Na_2HPO_4, sodium hydrogen phosphate	anti-caking agent; used in powdered products
Na_2SO_3, sodium sulfite	preservative

3.4.4: Compounds Containing a Metal Ion with a Variable Charge

Most of the transition metals and some main group metals can form two or more cations with different charges. Compounds of these metals with nonmetals are named with the same method as compounds in the first category, except the charge of the metal ion is specified by a Roman numeral in parentheses after the name of the metal. The charge of the metal ion is determined from the formula of the compound and the charge of the anion. For example, consider binary ionic compounds of iron and chlorine. Iron typically exhibits a charge of either 2+ or 3+ (see Figure 2.29), and the two corresponding compound formulas are $FeCl_2$ and $FeCl_3$. The simplest name, “iron chloride,” will, in this case, be ambiguous, as it does not distinguish between these two compounds. In cases like this, the charge of the metal ion is included as a Roman numeral in parentheses immediately following the metal name. These two compounds are then unambiguously named iron(II) chloride and iron(III) chloride, respectively. Other examples are provided in Table **3.4.4**.

Table **3.4.4**: Some Ionic Compounds with Variably Charged Metal Ions

Compound	Name
$FeCl_2$	iron(II) chloride
$FeCl_3$	iron(III) chloride
Hg_2O	mercury(I) oxide
HgO	mercury(II) oxide
SnF_2	tin(II) fluoride
SnF_4	tin(IV) fluoride

Out-of-date nomenclature used the suffixes *–ic* and *–ous* to designate metals with higher and lower charges, respectively: Iron(III) chloride, $FeCl_3$, was previously called ferric chloride, and iron(II) chloride, $FeCl_2$, was known as ferrous chloride. Though this naming convention has been largely abandoned by the scientific community, it remains in use by some segments of industry. For example, you may see the words *stannous fluoride* on a tube of toothpaste. This represents the formula SnF_2, which is more properly named tin(II) fluoride. The other fluoride of tin is SnF_4, which was previously called stannic fluoride but is now named tin(IV) fluoride.

3.4.5: Ionic Hydrates

Ionic compounds that contain water molecules as integral components of their crystals are called **hydrates**. The name for an ionic hydrate is derived by adding a term to the name for the anhydrous (meaning "not hydrated") compound that indicates the number of water molecules associated with each formula unit of the compound. The added word begins with a Greek prefix denoting the number of water molecules (see Table **3.4.5**) and ends with "hydrate." For example, the anhydrous compound copper(II) sulfate also exists as a hydrate containing five water molecules and named copper(II) sulfate pentahydrate. Washing soda is the common name for a hydrate of sodium carbonate containing 10 water molecules; the systematic name is sodium carbonate decahydrate.

Formulas for ionic hydrates are written by appending a vertically centered dot, a coefficient representing the number of water molecules, and the formula for water. The two examples mentioned in the previous paragraph are represented by the formulas

$$\text{copper(II) sulfate pentahydrate} \quad CuSO_4 \cdot 5H_2O$$

$$\text{sodium carbonate decahydrate} \quad Na_2CO_3 \cdot 10H_2O$$

Table **3.4.5**: Nomenclature Prefixes

Number	Prefix	Number	Prefix
1 (sometimes omitted)	mono-	6	hexa-
2	di-	7	hepta-
3	tri-	8	octa-
4	tetra-	9	nona-
5	penta-	10	deca-

Example **3.4.1**: Naming Ionic Compounds

Name the following ionic compounds

a. Fe_2S_3
b. CuSe
c. GaN
d. $MgSO_4 \cdot 7H_2O$
e. $Ti_2(SO_4)_3$

Solution

The anions in these compounds have a fixed negative charge (S^{2-}, Se^{2-} , N^{3-}, and and the compounds must be neutral. Because the total number of positive charges in each compound must equal the total number of negative charges, the positive ions must be Fe^{3+}, Cu^{2+}, Ga^{3+}, Mg^{2+}, and Ti^{3+}. These charges are used in the names of the metal ions:

a. iron(III) sulfide
b. copper(II) selenide
c. gallium(III) nitride
d. magnesium sulfate heptahydrate
e. titanium(III) sulfate

Exercise 3.4.1

Write the formulas of the following ionic compounds:

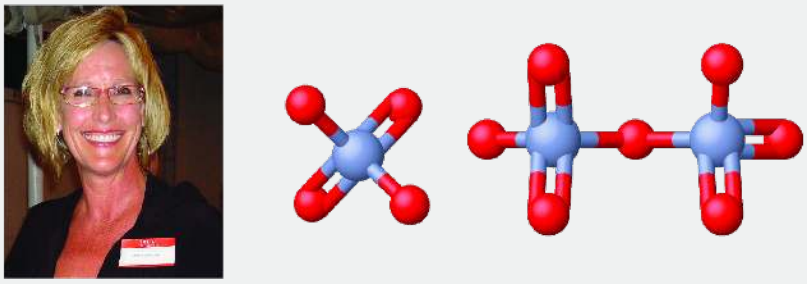
a. chromium(III) phosphide
b. mercury(II) sulfide
c. manganese(II) phosphate
d. copper(I) oxide
e. iron(III) chloride dihydrate

Answer

(a) CrP; (b) HgS; (c) $Mn_3(PO_4)_2$; (d) Cu_2O; (e) $FeCl_3 \cdot 2H_2O$

Chemistry in Everyday Life: Erin Brockovich and Chromium Contamination

In the early 1990s, legal file clerk Erin Brockovich (Figure **3.4.1**) discovered a high rate of serious illnesses in the small town of Hinckley, California. Her investigation eventually linked the illnesses to groundwater contaminated by Cr(VI) used by Pacific Gas & Electric (PG&E) to fight corrosion in a nearby natural gas pipeline. As dramatized in the film *Erin Brockovich* (for which Julia Roberts won an Oscar), Erin and lawyer Edward Masry sued PG&E for contaminating the water near Hinckley in 1993. The settlement they won in 1996—$333 million—was the largest amount ever awarded for a direct-action lawsuit in the US at that time.



(a) (b)

Figure **3.4.1**: (a) Erin Brockovich found that Cr(VI), used by PG&E, had contaminated the Hinckley, California, water supply. (b) The Cr(VI) ion is often present in water as the polyatomic ions chromate, (left), and dichromate, (right).

Chromium compounds are widely used in industry, such as for chrome plating, in dye-making, as preservatives, and to prevent corrosion in cooling tower water, as occurred near Hinckley. In the environment, chromium exists primarily in either the Cr(III) or Cr(VI) forms. Cr(III), an ingredient of many vitamin and nutritional supplements, forms compounds that are not very soluble in water, and it has low toxicity. But Cr(VI) is much more toxic and forms compounds that are reasonably soluble in water. Exposure to small amounts of Cr(VI) can lead to damage of the respiratory, gastrointestinal, and immune systems, as well as the kidneys, liver, blood, and skin.

Despite cleanup efforts, Cr(VI) groundwater contamination remains a problem in Hinckley and other locations across the globe. A 2010 study by the Environmental Working Group found that of 35 US cities tested, 31 had higher levels of Cr(VI) in their tap water than the public health goal of 0.02 parts per billion set by the California Environmental Protection Agency.

3.4.6: Molecular (Covalent) Compounds

The bonding characteristics of inorganic molecular compounds are different from ionic compounds, and they are named using a different system as well. The charges of cations and anions dictate their ratios in ionic compounds, so specifying the names of the ions provides sufficient information to determine chemical formulas. However, because covalent bonding allows for significant variation in the combination ratios of the atoms in a molecule, the names for molecular compounds must explicitly identify these ratios.

3.4.7: Compounds Composed of Two Elements

When two nonmetallic elements form a molecular compound, several combination ratios are often possible. For example, carbon and oxygen can form the compounds CO and CO_2. Since these are different substances with different properties, they cannot both have the same name (they cannot both be called carbon oxide). To deal with this situation, we use a naming method that is somewhat similar to that used for ionic compounds, but with added prefixes to specify the numbers of atoms of each element. The name of the more metallic element (the one farther to the left and/or bottom of the periodic table) is first, followed by the name of the more nonmetallic element (the one farther to the right and/or top) with its ending changed to the suffix *–ide*. The numbers of atoms of each element are designated by the Greek prefixes shown in Table **3.4.5**.

When only one atom of the first element is present, the prefix *mono-* is usually deleted from that part. Thus, CO is named carbon monoxide, and CO_2 is called carbon dioxide. When two vowels are adjacent, the *a* in the Greek prefix is usually dropped. Some other examples are shown in Table **3.4.6**.

Table **3.4.6**: Names of Some Molecular Compounds Composed of Two Elements

Compound	Name	Compound	Name
SO_2	sulfur dioxide	BCl_3	boron trichloride
SO_3	sulfur trioxide	SF_6	sulfur hexafluoride
NO_2	nitrogen dioxide	PF_5	phosphorus pentafluoride
N_2O_4	dinitrogen tetroxide	P_4O_{10}	tetraphosphorus decaoxide
N_2O_5	dinitrogen pentoxide	IF_7	iodine heptafluoride

There are a few common names that you will encounter as you continue your study of chemistry. For example, although NO is often called nitric oxide, its proper name is nitrogen monoxide. Similarly, N_2O is known as nitrous oxide even though our rules would specify the name dinitrogen monoxide. (And H_2O is usually called water, not dihydrogen monoxide.) You should commit to memory the common names of compounds as you encounter them.

✔ Example **3.4.2**: Naming Covalent Compounds

Name the following covalent compounds:

a. SF_6
b. N_2O_3
c. Cl_2O_7
d. P_4O_6

Solution

Because these compounds consist solely of nonmetals, we use prefixes to designate the number of atoms of each element:

a. sulfur hexafluoride
b. dinitrogen trioxide
c. dichlorine heptoxide
d. tetraphosphorus hexoxide

? Exercise **3.4.2**

Write the formulas for the following compounds:

a. phosphorus pentachloride
b. dinitrogen monoxide
c. iodine heptafluoride
d. carbon tetrachloride

Answer

(a) PCl_5; (b) N_2O; (c) IF_7; (d) CCl_4

Link to Learning

The following website provides practice with naming chemical compounds and writing chemical formulas. You can choose binary, polyatomic, and variable charge ionic compounds, as well as molecular compounds.

3.4.8: Binary Acids

Some compounds containing hydrogen are members of an important class of substances known as **acids**. The chemistry of these compounds is explored in more detail in later chapters of this text, but for now, it will suffice to note that many acids release hydrogen ions, H^+, when dissolved in water. To denote this distinct chemical property, a mixture of water with an acid is given a name derived from the compound's name. If the compound is a binary acid (comprised of hydrogen and one other nonmetallic element):

1. The word "hydrogen" is changed to the prefix *hydro-*
2. The other nonmetallic element name is modified by adding the suffix *-ic*
3. The word "acid" is added as a second word

For example, when the gas HCl (hydrogen chloride) is dissolved in water, the solution is called *hydrochloric acid*. Several other examples of this nomenclature are shown in Table **3.4.7**.

Table **3.4.7**: Names of Some Simple Acids

Name of Gas	Name of Acid
HF(*g*), hydrogen fluoride	HF(*aq*), hydrofluoric acid
HCl(*g*), hydrogen chloride	HCl(*aq*), hydrochloric acid
HBr(*g*), hydrogen bromide	HBr(*aq*), hydrobromic acid
HI(*g*), hydrogen iodide	HI(*aq*), hydroiodic acid
H_2S(*g*), hydrogen sulfide	H_2S(*aq*), hydrosulfuric acid

3.4.9: Oxyacids

Many compounds containing three or more elements (such as organic compounds or coordination compounds) are subject to specialized nomenclature rules that you will learn later. However, we will briefly discuss the important compounds known as **oxyacids**, compounds that contain hydrogen, oxygen, and at least one other element, and are bonded in such a way as to impart acidic properties to the compound (you will learn the details of this in a later chapter). Typical oxyacids consist of hydrogen combined with a polyatomic, oxygen-containing ion. To name oxyacids:

1. Omit "hydrogen"
2. Start with the root name of the anion
3. Replace *–ate* with *–ic*, or *–ite* with *–ous*
4. Add "acid"

For example, consider H_2CO_3 (which you might be tempted to call "hydrogen carbonate"). To name this correctly, "hydrogen" is omitted; the *–ate* of carbonate is replace with *–ic*; and acid is added—so its name is carbonic acid. Other examples are given in Table **3.4.8**. There are some exceptions to the general naming method (e.g., H_2SO_4 is called sulfuric acid, not sulfic acid, and H_2SO_3 is sulfurous, not sulfous, acid).

Table **3.4.8**: Names of Common Oxyacids

Formula	Anion Name	Acid Name
$HC_2H_3O_2$	acetate	acetic acid
HNO_3	nitrate	nitric acid
HNO_2	nitrite	nitrous acid
$HClO_4$	perchlorate	perchloric acid
H_2CO_3	carbonate	carbonic acid
H_2SO_4	sulfate	sulfuric acid
H_2SO_3	sulfite	sulfurous acid
H_3PO_4	phosphate	phosphoric acid

This page titled 3.4: Chemical Nomenclature is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **2.7: Chemical Nomenclature** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

3.5: Case Study- Ionic and Covalent Compounds in Biochemistry

Introduction: In the realm of organic and inorganic biochemistry, the nuanced interplay between ionic and covalent compounds forms the cornerstone of countless biochemical processes. This case study peers into the practical application of these compounds in medical treatments, specifically through the lens of a pharmacist crafting a life-saving electrolyte solution for a dehydrated patient.

Scenario: Pharmacist Dr. Laura Hernandez faces a challenge: her patient, Michael, has arrived at the emergency room severely dehydrated. To stabilize his condition, she must formulate an electrolyte solution that precisely mimics the electrolyte balance of the human body. Her deep understanding of the properties of ionic and covalent compounds is critical in concocting a remedy that not only rehydrates but also ensures compatibility with Michael's physiological processes.

Ionic vs. Covalent Compounds: Dr. Hernandez knows that ionic compounds, with their capacity to break down into ions in solution, are perfect for rapidly replenishing Michael's depleted electrolytes. Covalent compounds, which form molecules through shared electrons, won't dissociate in the same way but play a different, equally crucial role in the body's chemistry and in drug efficacy.

Case Study Questions:

1. **Compare and contrast ionic and covalent compounds.**
2. **How do covalent bonds affect drug interactions with enzymes?**

Hands-On Classroom Activities:

1. **Build a Model:** In the "Build a Model" activity, students will employ marshmallows and toothpicks to construct tangible models of atoms. Through this creative process, they will demonstrate the concept of electron shells and the specific electrons involved in bonding, known as valence electrons. This hands-on activity is designed to enhance students' understanding of atomic structure and electron configuration.
2. **Research Discussion:** The "Research Discussion" activity involves students conducting in-depth explorations into the latest advancements in radiation therapy. Following their research, students will present their findings on how the knowledge of electron movement is essential in developing current treatment strategies. This discussion aims to connect theoretical electron dynamics with practical applications in medical treatments.

Conclusion: Through her skillful application of biochemistry, Dr. Hernandez not only stabilizes Michael but also serves as a conduit for medical students to witness the profound impact of ionic and covalent compounds in clinical practice. This case study exemplifies the vital role of biochemical knowledge in developing therapeutic strategies, illuminating the intricate dance between chemical structure and biological function that defines the field of biochemistry.

3.5: Case Study- Ionic and Covalent Compounds in Biochemistry is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

3.E: Exercises

Multiple-Choice Questions

1. Which atom is likely to form a cation?
   a. O
   b. Ar
   c. Br
   d. K
2. Which is not a physical property of metals?
   a. Good conductor of heat
   b. Good insulator of electricity
   c. Malleable
   d. Ductile
3. What is the charge on sulfate?
   a. +1
   b. 0
   c. −1
   d. −2
4. Which element is a nonmetal?
   a. Li
   b. S
   c. Ca
   d. Zn
5. What is the correct chemical formula for the ionic compound formed between calcium and oxygen?
   a. CaO
   b. Ca_2O
   c. CaO_2
   d. Ca_2O_2
6. What is the correct name of AlP?
   a. aluminum phosphide
   b. aluminum(III) phosphide
   c. aluminum phosphite
   d. aluminum phosphate
7. What is the correct name of P_2O_5?
   a. phosphorus oxide
   b. diphosphorus pentoxide
   c. diphosphorus oxide

d. phosphorus pentoxide

8. What is the correct formula for nitrous acid?

a. HN_3

b. HNO

c. HNO_2

d. HNO_3

9. What is the correct name of Cr_2S_3?

a. chromium sulfide

b. dichromium trisulfide

c. chromium(II) sulfide

d. chromium(III) sulfide

10. What is the correct formula for ammonium sulfate?

a. NH_4SO_3

b. NH_4SO_4

c. $(NH_4)_2SO_3$

d. $(NH_4)_2SO_4$

Warm-up Problems

1. Which of the following common biological ions are metals?

Cations: sodium, potassium, calcium, magnesium

Anions: chloride, hydroxide, bicarbonate, hydrogen phosphate, dihydrogen phosphate

2. Which of the following common biological ions contain non-metals? Also, assign their charges.

Cations: sodium, potassium, calcium, magnesium

Anions: chloride, hydroxide, bicarbonate, hydrogen phosphate, dihydrogen phosphate

3. Which is likely to form a cation: lithium or fluorine?

4. Which is likely to form an anion: aluminum or oxygen?

5. What is the formula for an ionic compound formed from Mg^{2+} and Cl^{-}?

6. What is the formula for an ionic compound formed from Na^{+} and S^{2-}?

7. Some substances can conduct electricity. Is conductivity a physical or a chemical property? Is this property associated with metals or nonmetals?

8. Arsenic is known to be toxic when ingested. Is this a physical or a chemical property of arsenic?

9. What is the most common charge on magnesium in an ionic compound?

10. What is the most common charge on oxygen in an ionic compound?

11. Is CCl_4 an ionic or covalent compound?

12. Is LiF an ionic or covalent compound?

Problems

1. Name the following compounds
    a. CsCl
    b. BaO
2. Name the following compounds
    a. K_2S
    b. $BeCl_2$
3. Name the following compounds
    a. HBr
    b. AlF_3
4. Name the following compounds
    a. NaF
    b. Rb_2O
5. Name the following compounds
    a. BCl_3
    b. H_2Se
6. Name the following compounds
    a. P_4O_6
    b. ICl_3
7. Write the formulas for the following compounds:
    a. chlorine dioxide
    b. dinitrogen tetroxide
    c. potassium phosphide
8. Write the formulas for the following compounds:
    a. silver sulfide
    b. aluminum nitride
    c. silicon dioxide
9. Write the formulas for the following compounds:
    a. barium chloride
    b. magnesium nitride
    c. sulfur dioxide
10. Write the formulas for the following compounds:
    a. nitrogen trichloride
    b. dinitrogen trioxide
    c. tin(IV) chloride
11. Each of the following compounds contains a metal that can exhibit more than one ionic charge. Name these compounds:
    a. Cr_2O_3
    b. $FeCl_2$

c. CrO_3

12. Each of the following compounds contains a metal that can exhibit more than one ionic charge. Name these compounds:
    a. $TiCl_4$
    b. CoO
    c. MoS_2
13. Each of the following compounds contains a metal that can exhibit more than one ionic charge. Name these compounds:
    a. $NiCO_3$
    b. MoO_3
    c. $Co(NO_3)_2$
14. Each of the following compounds contains a metal that can exhibit more than one ionic charge. Name these compounds:
    a. V_2O_5
    b. MnO_2
    c. Fe_2O_3
15. The following ionic compounds are found in common household products. Write the formula for each compound:
    a. potassium phosphate
    b. copper(II) sulfate
    c. calcium chloride
16. The following ionic compounds are found in common household products. Write the formula for each compound:
    a. titanium(IV) oxide
    b. ammonium nitrate
    c. sodium hydrogen sulfate
17. The following ionic compounds are found in common household products. Name each of the compounds:
    a. $Ca(H_2PO_4)_2$
    b. $FeSO_4$
    c. $CaCO_3$
18. The following ionic compounds are found in common household products. Name each of the compounds:
    a. MgO
    b. $NaNO_2$
    c. KI

Challenge Problems

1. A binary ionic compound has the formula X_2Y_3, where X and Y are different elements. Provide two possible chemical formulas for this compound. (revise to make this better)
2. Iron is an important mineral, and those with anemia (iron deficiency), can take supplements to treat the deficiency. A common ingredient in iron supplements is $FeSO_4$. What is the proper IUPAC name for this ionic compound? What are the charges on the ions?
3. Iron is an important mineral, and those with anemia (iron deficiency), can take supplements to treat the deficiency. One possible ingredient in iron supplements is $Fe_2(SO_4)_3$. What is the proper IUPAC name for this ionic compound? What are the charges on the ions?

Health-Related Problems

1. Kidney stones are a mixture of various materials including calcium oxalate and calcium phosphate, among other species. What are the molecular formulas for these two species and are they ionic or covalent? Oxalate is a $C_2O_4^{2-}$ dianion that is high in some foods such as spinach. Most people can eat high oxalate foods with no problem, but those who have a high predisposition to form kidney stones might want to avoid those foods.
2. Iron supplements for those with anemia (iron deficiency) often contain a compound called “ferrous sulfate”. “Ferrous” is an old term for iron(II). What is the molecular formula for ferrous sulfate?

3.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

4: Chemical Bonding

4.1: Lewis Symbols and Structures
4.2: Formal Charges and Resonance
4.3: Molecular Structure and Polarity
4.4: Valence Bond Theory
4.5: Hybrid Atomic Orbitals
4.6: Multiple Bonds
4.7: Case Study- Chemical Bonding - Deciphering Drug Interactions through Lewis Structures
4.8: 3D Printing Activity- VSEPR and Ionic/Metallic Solids Structures
4.E: Exercises

4: Chemical Bonding is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

4.1: Lewis Symbols and Structures

Learning Objectives

By the end of this section, you will be able to:

- Write Lewis symbols for neutral atoms and ions
- Draw Lewis structures depicting the bonding in simple molecules

Thus far in this chapter, we have discussed the various types of bonds that form between atoms and/or ions. In all cases, these bonds involve the sharing or transfer of valence shell electrons between atoms. In this section, we will explore the typical method for depicting valence shell electrons and chemical bonds, namely Lewis symbols and Lewis structures.

4.1.1: Lewis Symbols

We use Lewis symbols to describe valence electron configurations of atoms and monatomic ions. A Lewis symbol consists of an elemental symbol surrounded by one dot for each of its valence electrons:



Figure **4.1.1**: shows the Lewis symbols for the elements of the third period of the periodic table.

Atoms	Electronic Configuration	Lewis Symbol
sodium	$[Ne]3s^1$	Na·
magnesium	$[Ne]3s^2$	·Mg·
aluminum	$[Ne]3s^23p^1$	·Al·
silicon	$[Ne]3s^23p^2$	·Si·
phosphorus	$[Ne]3s^23p^3$	·P·
sulfur	$[Ne]3s^23p^4$	:S·
chlorine	$[Ne]3s^23p^5$	:Cl·
argon	$[Ne]3s^23p^6$	:Ar:

Figure **4.1.1**: Lewis symbols illustrating the number of valence electrons for each element in the third period of the periodic table.

Lewis symbols can also be used to illustrate the formation of cations from atoms, as shown here for sodium and calcium:



Likewise, they can be used to show the formation of anions from atoms, as shown here for chlorine and sulfur:



Figure **4.1.2** demonstrates the use of Lewis symbols to show the transfer of electrons during the formation of ionic compounds.

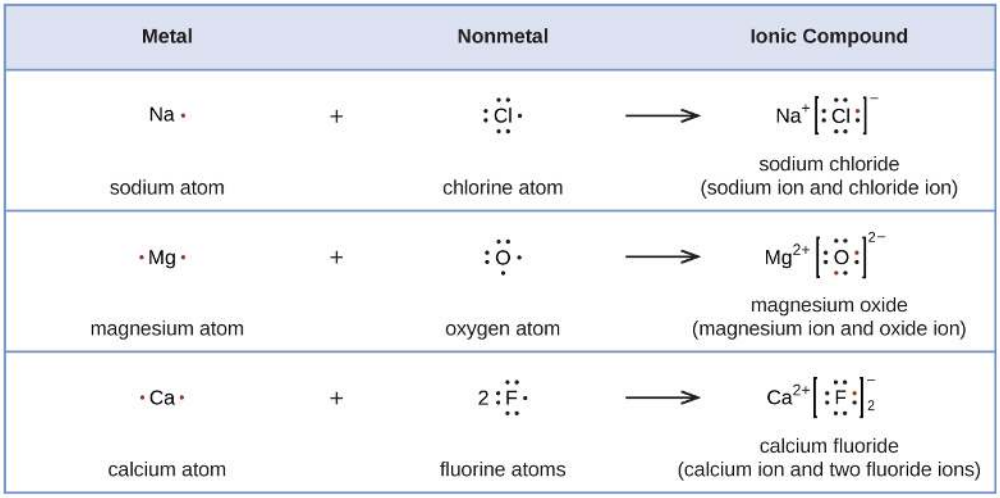
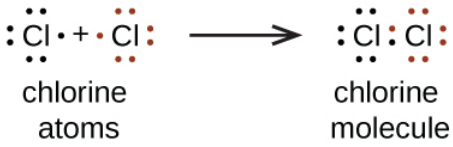


Figure **4.1.2**: Cations are formed when atoms lose electrons, represented by fewer Lewis dots, whereas anions are formed by atoms gaining electrons. The total number of electrons does not change.

4.1.2: Lewis Structures

We also use Lewis symbols to indicate the formation of covalent bonds, which are shown in Lewis structures, drawings that describe the bonding in molecules and polyatomic ions. For example, when two chlorine atoms form a chlorine molecule, they share one pair of electrons:



The Lewis structure indicates that each Cl atom has three pairs of electrons that are not used in bonding (called lone pairs) and one shared pair of electrons (written between the atoms). A dash (or line) is sometimes used to indicate a shared pair of electrons:

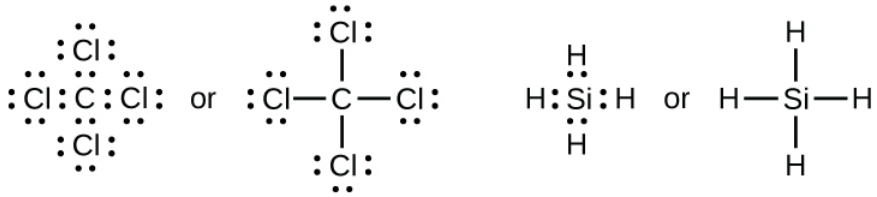


A single shared pair of electrons is called a single bond. Each Cl atom interacts with eight valence electrons: the six in the lone pairs and the two in the single bond.

4.1.2.1: The Octet Rule

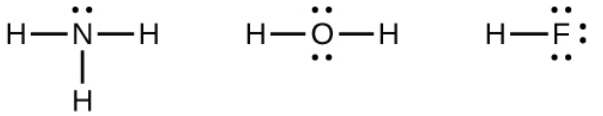
The other halogen molecules (F_2, Br_2, I_2, and At_2) form bonds like those in the chlorine molecule: one single bond between atoms and three lone pairs of electrons per atom. This allows each halogen atom to have a noble gas electron configuration. The tendency of main group atoms to form enough bonds to obtain eight valence electrons is known as the octet rule.

The number of bonds that an atom can form can often be predicted from the number of electrons needed to reach an octet (eight valence electrons); this is especially true of the nonmetals of the second period of the periodic table (C, N, O, and F). For example, each atom of a group 14 element has four electrons in its outermost shell and therefore requires four more electrons to reach an octet. These four electrons can be gained by forming four covalent bonds, as illustrated here for carbon in CCl_4 (carbon tetrachloride) and silicon in SiH_4 (silane). Because hydrogen only needs two electrons to fill its valence shell, it is an exception to the octet rule. The transition elements and inner transition elements also do not follow the octet rule:



carbon tetrachloride silane

Group 15 elements such as nitrogen have five valence electrons in the atomic Lewis symbol: one lone pair and three unpaired electrons. To obtain an octet, these atoms form three covalent bonds, as in NH_3 (ammonia). Oxygen and other atoms in group 16 obtain an octet by forming two covalent bonds:



ammonia Water hydrogen fluoride

4.1.2.2: Double and Triple Bonds

As previously mentioned, when a pair of atoms shares one pair of electrons, we call this a single bond. However, a pair of atoms may need to share more than one pair of electrons in order to achieve the requisite octet. A double bond forms when two pairs of electrons are shared between a pair of atoms, as between the carbon and oxygen atoms in CH_2O (formaldehyde) and between the two carbon atoms in C_2H_4 (ethylene):



formaldehyde ethylene

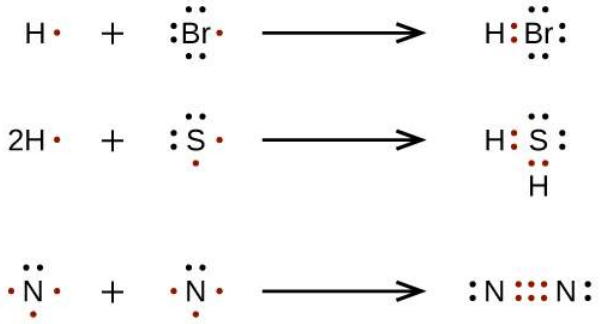
A triple bond forms when three electron pairs are shared by a pair of atoms, as in carbon monoxide (CO) and the cyanide ion (CN^-):



carbon monoxide cyanide ion

4.1.3: Writing Lewis Structures with the Octet Rule

For very simple molecules and molecular ions, we can write the Lewis structures by merely pairing up the unpaired electrons on the constituent atoms. See these examples:



For more complicated molecules and molecular ions, it is helpful to follow the step-by-step procedure outlined here.

Writing Lewis Structures

1. Determine the total number of valence (outer shell) electrons. For cations, subtract one electron for each positive charge. For anions, add one electron for each negative charge.
2. Draw a skeleton structure of the molecule or ion, arranging the atoms around a central atom. (Generally, the least electronegative element should be placed in the center.) Connect each atom to the central atom with a single bond (one electron pair).
3. Distribute the remaining electrons as lone pairs on the terminal atoms (except hydrogen), completing an octet around each atom.
4. Place all remaining electrons on the central atom.
5. Rearrange the electrons of the outer atoms to make multiple bonds with the central atom in order to obtain octets wherever possible.

Let us determine the Lewis structures of $\mathbf{SiH_4}$, $\mathbf{CHO_2^-}$, $\mathbf{NO^+}$, and $\mathbf{OF_2}$ as examples in following this procedure:

1. Determine the total number of valence (outer shell) electrons in the molecule or ion.
   - For a molecule, we add the number of valence electrons on each atom in the molecule:

$$\begin{array}{r} \mathbf{SiH_4} \\ \mathbf{Si:\ 4\ valence\ electrons/atom \times\ 1\ atom\ = 4} \\ \mathbf{+\quad H:\ 1\ valence\ electron/atom \times\ 4\ atoms = 4} \\ \hline \mathbf{total\ valence\ electrons = 8} \end{array}$$

   - For a *negative ion*, such as $\mathbf{CHO_2^-}$, we add the number of valence electrons on the atoms to the number of negative charges on the ion (one electron is gained for each single negative charge):

$$\begin{array}{r} \mathbf{CHO_2^-} \\ \mathbf{C:\ 4\ valence\ electrons/atom \times\ 1\ atom\ = 4} \\ \mathbf{H:\ 1\ valence\ electron/atom \times\ 1\ atoms = 1} \\ \mathbf{O:\ 6\ valence\ electron/atom \times\ 2\ atoms = 12} \\ \mathbf{+\quad 1\ electron = 1} \\ \hline \mathbf{total\ valence\ electrons = 18} \end{array}$$

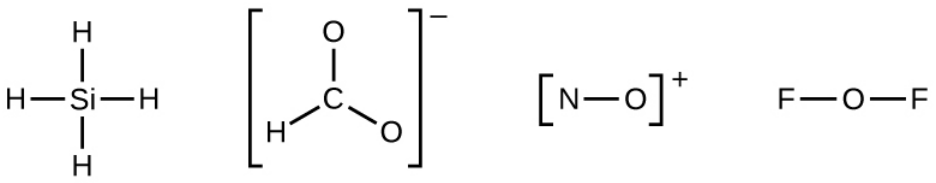
   - For a *positive ion*, such as $\mathbf{NO^+}$, we add the number of valence electrons on the atoms in the ion and then subtract the number of positive charges on the ion (one electron is lost for each single positive charge) from the total number of valence electrons:

$$\begin{array}{r} \mathrm{NO^+} \\ \text{N: 5 valence electrons/atom} \times \text{ 1 atom } = 5 \\ \text{O: 6 valence electron/atom} \times \text{ 1 atoms} = 6 \\ + \quad \text{e: -1 electron (positive charge)} \times \text{ 1 electron} = -1 \\ \hline \text{total valence electrons} = 10 \end{array}$$

- Since $\mathrm{OF_2}$ is a neutral molecule, we simply add the number of valence electrons:

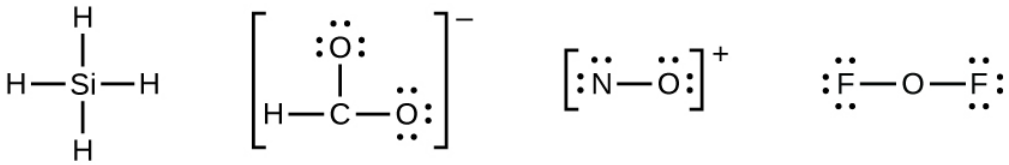
$$\begin{array}{r} \mathrm{OF_2} \\ \text{O: 6 valence electrons/atom} \times \text{ 1 atom } = 6 \\ + \quad \text{F: 7 valence electron/atom} \times \text{ 2 atoms} = 14 \\ \hline \text{total valence electrons} = 20 \end{array}$$

2. Draw a skeleton structure of the molecule or ion, arranging the atoms around a central atom and connecting each atom to the central atom with a single (one electron pair) bond. (Note that we denote ions with brackets around the structure, indicating the charge outside the brackets:)

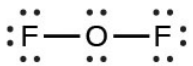


When several arrangements of atoms are possible, as for $\mathrm{CHO_2^-}$, we must use experimental evidence to choose the correct one. In general, the less electronegative elements are more likely to be central atoms. In $\mathrm{CHO_2^-}$, the less electronegative carbon atom occupies the central position with the oxygen and hydrogen atoms surrounding it. Other examples include P in $\mathrm{POCl_3}$, S in $\mathrm{SO_2}$, and Cl in $\mathrm{ClO_4^-}$. An exception is that hydrogen is almost never a central atom. As the most electronegative element, fluorine also cannot be a central atom.

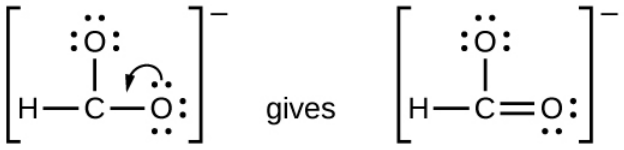
3. Distribute the remaining electrons as lone pairs on the terminal atoms (except hydrogen) to complete their valence shells with an octet of electrons.
   - There are no remaining electrons on $\mathrm{SiH_4}$, so it is unchanged:



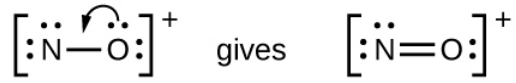
4. Place all remaining electrons on the central atom.
   - For $\mathrm{SiH_4}$, $\mathrm{CHO_2^-}$, and $\mathrm{NO^+}$, there are no remaining electrons; we already placed all of the electrons determined in Step 1.
   - For $\mathrm{OF_2}$, we had 16 electrons remaining in Step 3, and we placed 12, leaving 4 to be placed on the central atom:



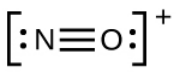
5. Rearrange the electrons of the outer atoms to make multiple bonds with the central atom in order to obtain octets wherever possible.
   - $\mathrm{SiH_4}$: Si already has an octet, so nothing needs to be done.
   - $\mathrm{CHO\ 2^-}$: We have distributed the valence electrons as lone pairs on the oxygen atoms, but the carbon atom lacks an octet:



- NO^+: For this ion, we added eight valence electrons, but neither atom has an octet. We cannot add any more electrons since we have already used the total that we found in Step 1, so we must move electrons to form a multiple bond:



This still does not produce an octet, so we must move another pair, forming a triple bond:



- In OF_2, each atom has an octet as drawn, so nothing changes.

Example 4.1.1: Writing Lewis Structures

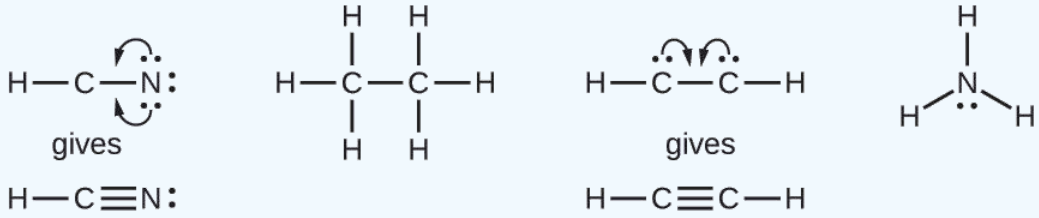
NASA's Cassini-Huygens mission detected a large cloud of toxic hydrogen cyanide (HCN) on Titan, one of Saturn's moons. Titan also contains ethane (H_3CCH_3), acetylene (HCCH), and ammonia (NH_3). What are the Lewis structures of these molecules?

Solution

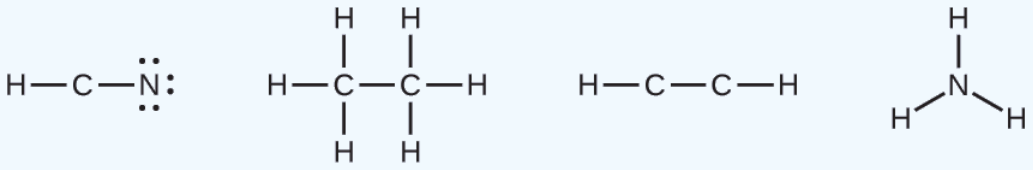
Step 1. *Calculate the number of valence electrons.*

HCN: (1 × 1) + (4 × 1) + (5 × 1) = 10
H_3CCH_3: (1 × 3) + (2 × 4) + (1 × 3) = 14
HCCH: (1 × 1) + (2 × 4) + (1 × 1) = 10
NH_3: (5 × 1) + (3 × 1) = 8

Step 2 *Draw a skeleton and connect the atoms with single bonds.* Remember that H is never a central atom:

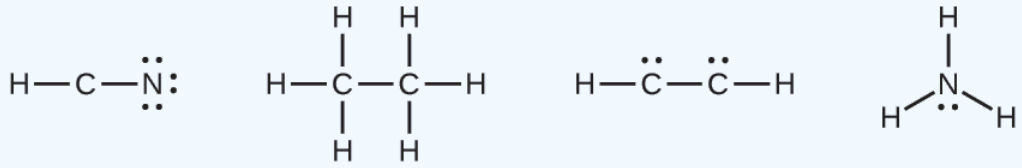


Step 3. *Where needed, distribute electrons to the terminal atoms:*



HCN: six electrons placed on N
H_3CCH_3: no electrons remain
HCCH: no terminal atoms capable of accepting electrons
NH_3: no terminal atoms capable of accepting electrons

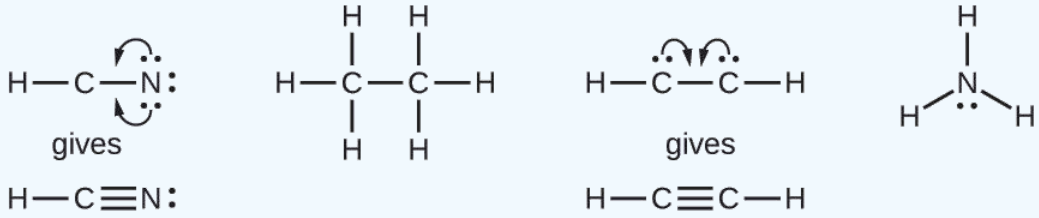
Step 4. *Where needed, place remaining electrons on the central atom:*



HCN: no electrons remain
H_3CCH_3: no electrons remain
HCCH: four electrons placed on carbon
NH_3: two electrons placed on nitrogen

Step 5. *Where needed, rearrange electrons to form multiple bonds in order to obtain an octet on each atom:*

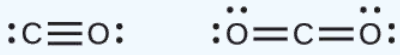
HCN: form two more C–N bonds
H_3CCH_3: all atoms have the correct number of electrons
HCCH: form a triple bond between the two carbon atoms
NH_3: all atoms have the correct number of electrons



Exercise 4.1.1

Both carbon monoxide, CO, and carbon dioxide, CO_2, are products of the combustion of fossil fuels. Both of these gases also cause problems: CO is toxic and CO_2 has been implicated in global climate change. What are the Lewis structures of these two molecules?

Answer



How Sciences Interconnect: Fullerene Chemistry

Carbon, in various forms and compounds, has been known since prehistoric times, . Soot has been used as a pigment (often called carbon black) for thousands of years. Charcoal, high in carbon content, has likewise been critical to human development. Carbon is the key additive to iron in the steelmaking process, and diamonds have a unique place in both culture and industry. With all this usage came significant study, particularly with the emergence of organic chemistry. And even with all the known forms and functions of the element, scientists began to uncover the potential for even more varied and extensive carbon structures.

As early as the 1960s, chemists began to observe complex carbon structures, but they had little evidence to support their concepts, or their work did not make it into the mainstream. Eiji Osawa predicted a spherical form based on observations of a similar structure, but his work was not widely known outside Japan. In a similar manner, the most comprehensive advance was likely computational chemist Elena Galpern's, who in 1973 predicted a highly stable, 60-carbon molecule; her work was also isolated to her native Russia. Still later, Harold Kroto, working with Canadian radio astronomers, sought to uncover the nature of long carbon chains that had been discovered in interstellar space.

Kroto sought to use a machine developed by Richard Smalley's team at Rice University to learn more about these structures. Together with Robert Curl, who had introduced them, and three graduate students—James Heath, Sean O'Brien, and Yuan Liu—they performed an intensive series of experiments that led to a major discovery.

In 1996, the Nobel Prize in Chemistry was awarded to Richard Smalley (Figure **4.1.3**), Robert Curl, and Harold Kroto for their work in discovering a new form of carbon, the C_{60} buckminsterfullerene molecule. An entire class of compounds, including spheres and tubes of various shapes, were discovered based on C_{60}. This type of molecule, called a fullerene, shows promise in a variety of applications. Because of their size and shape, fullerenes can encapsulate other molecules, so they have shown potential in various applications from hydrogen storage to targeted drug delivery systems. They also possess unique electronic and optical properties that have been put to good use in solar powered devices and chemical sensors.

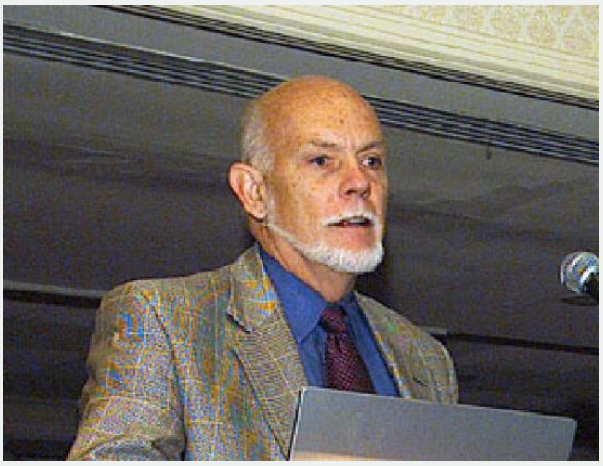


Figure **4.1.3**: Richard Smalley (1943–2005), a professor of physics, chemistry, and astronomy at Rice University, was one of the leading advocates for fullerene chemistry. Upon his death in 2005, the US Senate honored him as the "Father of Nanotechnology." (credit: United States Department of Energy)

4.1.4: Exceptions to the Octet Rule

Many covalent molecules have central atoms that do not have eight electrons in their Lewis structures. These molecules fall into three categories:

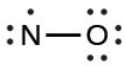
- Odd-electron molecules have an odd number of valence electrons, and therefore have an unpaired electron.
- Electron-deficient molecules have a central atom that has fewer electrons than needed for a noble gas configuration.
- Hypervalent molecules have a central atom that has more electrons than needed for a noble gas configuration.

4.1.4.1: Odd-electron Molecules

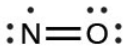
We call molecules that contain an odd number of electrons free radicals. Nitric oxide, NO, is an example of an odd-electron molecule; it is produced in internal combustion engines when oxygen and nitrogen react at high temperatures.

To draw the Lewis structure for an odd-electron molecule like NO, we follow the same five steps we would for other molecules, but with a few minor changes:

1. *Determine the total number of valence (outer shell) electrons*. The sum of the valence electrons is 5 (from N) + 6 (from O) = 11. The odd number immediately tells us that we have a free radical, so we know that not every atom can have eight electrons in its valence shell.
2. *Draw a skeleton structure of the molecule*. We can easily draw a skeleton with an N–O single bond:
   N–O
3. *Distribute the remaining electrons as lone pairs on the terminal atoms*. In this case, there is no central atom, so we distribute the electrons around both atoms. We give eight electrons to the more electronegative atom in these situations; thus oxygen has the filled valence shell:

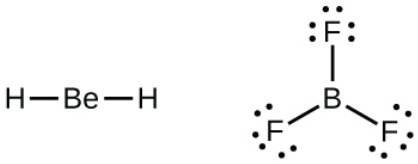


4. *Place all remaining electrons on the central atom.* Since there are no remaining electrons, this step does not apply.
5. *Rearrange the electrons to make multiple bonds with the central atom in order to obtain octets wherever possible.* We know that an odd-electron molecule cannot have an octet for every atom, but we want to get each atom as close to an octet as possible. In this case, nitrogen has only five electrons around it. To move closer to an octet for nitrogen, we take one of the lone pairs from oxygen and use it to form a NO double bond. (We cannot take another lone pair of electrons on oxygen and form a triple bond because nitrogen would then have nine electrons:)

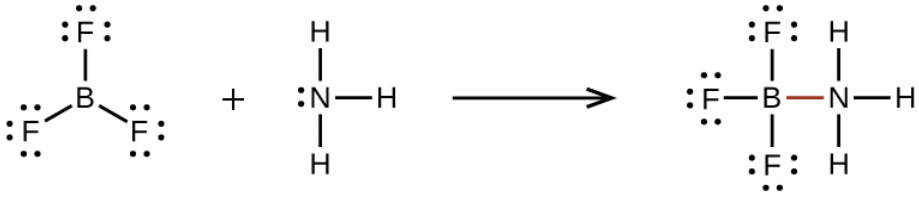


4.1.4.2: Electron-deficient Molecules

We will also encounter a few molecules that contain central atoms that do not have a filled valence shell. Generally, these are molecules with central atoms from groups 2 and 13, outer atoms that are hydrogen, or other atoms that do not form multiple bonds. For example, in the Lewis structures of beryllium dihydride, BeH_2, and boron trifluoride, BF_3, the beryllium and boron atoms each have only four and six electrons, respectively. It is possible to draw a structure with a double bond between a boron atom and a fluorine atom in BF_3, satisfying the octet rule, but experimental evidence indicates the bond lengths are closer to that expected for B–F single bonds. This suggests the best Lewis structure has three B–F single bonds and an electron deficient boron. The reactivity of the compound is also consistent with an electron deficient boron. However, the B–F bonds are slightly shorter than what is actually expected for B–F single bonds, indicating that some double bond character is found in the actual molecule.



An atom like the boron atom in BF_3, which does not have eight electrons, is very reactive. It readily combines with a molecule containing an atom with a lone pair of electrons. For example, NH_3 reacts with BF_3 because the lone pair on nitrogen can be shared with the boron atom:



4.1.4.3: Hypervalent Molecules

Elements in the second period of the periodic table ($n = 2$) can accommodate only eight electrons in their valence shell orbitals because they have only four valence orbitals (one 2*s* and three 2*p* orbitals). Elements in the third and higher periods ($n \geq 3$) have more than four valence orbitals and can share more than four pairs of electrons with other atoms because they have empty *d* orbitals in the same shell. Molecules formed from these elements are sometimes called hypervalent molecules. Figure **4.1.4**: shows the Lewis structures for two hypervalent molecules, PCl_5 and SF_6.

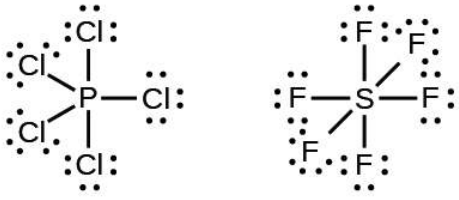
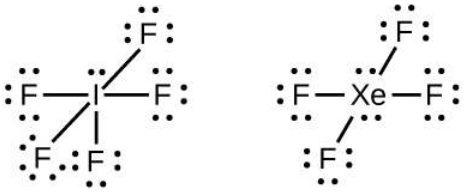


Figure **4.1.4**: In PCl_5, the central atom phosphorus shares five pairs of electrons. In SF_6, sulfur shares six pairs of electrons.

In some hypervalent molecules, such as IF_5 and XeF_4, some of the electrons in the outer shell of the central atom are lone pairs:



When we write the Lewis structures for these molecules, we find that we have electrons left over after filling the valence shells of the outer atoms with eight electrons. These additional electrons must be assigned to the central atom.

Example 4.1.2: Writing Lewis Structures - Octet Rule Violations

Xenon is a noble gas, but it forms a number of stable compounds. We examined XeF_4 earlier. What are the Lewis structures of XeF_2 and XeF_6?

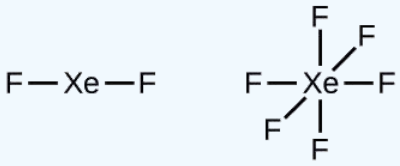
Solution

We can draw the Lewis structure of any covalent molecule by following the six steps discussed earlier. In this case, we can condense the last few steps, since not all of them apply.

Step 1. Calculate the number of valence electrons:

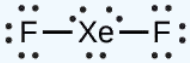
XeF_2: $8 + (2 \times 7) = 22$
XeF_6: $8 + (6 \times 7) = 50$

Step 2. Draw a skeleton joining the atoms by single bonds. Xenon will be the central atom because fluorine cannot be a central atom:

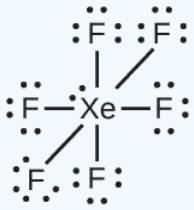


Step 3. Distribute the remaining electrons.

XeF_2: We place three lone pairs of electrons around each F atom, accounting for 12 electrons and giving each F atom 8 electrons. Thus, six electrons (three lone pairs) remain. These lone pairs must be placed on the Xe atom. This is acceptable because Xe atoms have empty valence shell *d* orbitals and can accommodate more than eight electrons. The Lewis structure of XeF_2 shows two bonding pairs and three lone pairs of electrons around the Xe atom:



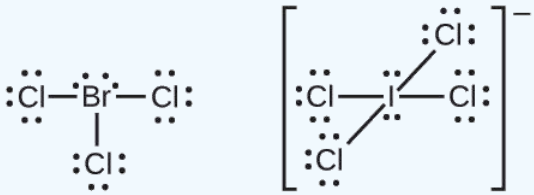
XeF_6: We place three lone pairs of electrons around each F atom, accounting for 36 electrons. Two electrons remain, and this lone pair is placed on the Xe atom:



Exercise 4.1.2: Interhalogens

The halogens form a class of compounds called the interhalogens, in which halogen atoms covalently bond to each other. Write the Lewis structures for the interhalogens $BrCl_3$ and ICl_4^-.

Answer



This page titled 4.1: Lewis Symbols and Structures is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **7.3: Lewis Symbols and Structures** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

4.2: Formal Charges and Resonance

Learning Objectives

By the end of this section, you will be able to:

- Compute formal charges for atoms in any Lewis structure
- Use formal charges to identify the most reasonable Lewis structure for a given molecule
- Explain the concept of resonance and draw Lewis structures representing resonance forms for a given molecule

In the previous section, we discussed how to write Lewis structures for molecules and polyatomic ions. As we have seen, however, in some cases, there is seemingly more than one valid structure for a molecule. We can use the concept of formal charges to help us predict the most appropriate Lewis structure when more than one is reasonable.

4.2.1: Calculating Formal Charge

The formal charge of an atom in a molecule is the *hypothetical* charge the atom would have if we could redistribute the electrons in the bonds evenly between the atoms. Another way of saying this is that formal charge results when we take the number of valence electrons of a neutral atom, subtract the nonbonding electrons, and then subtract the number of bonds connected to that atom in the Lewis structure.

Thus, we calculate formal charge as follows:

$$\text{formal charge } = \#\text{ valence shell electrons (free atom) } - \#\text{ lone pair electrons } - \frac{1}{2}\#\text{ bonding electrons}$$

We can double-check formal charge calculations by determining the sum of the formal charges for the whole structure. The sum of the formal charges of all atoms in a molecule must be zero; the sum of the formal charges in an ion should equal the charge of the ion.

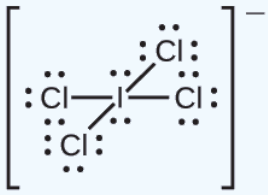
We must remember that the formal charge calculated for an atom is not the *actual* charge of the atom in the molecule. Formal charge is only a useful bookkeeping procedure; it does not indicate the presence of actual charges.

Example 4.2.1: Calculating Formal Charge from Lewis Structures

Assign formal charges to each atom in the interhalogen ion

Solution

Step 1. *We divide the bonding electron pairs equally for all I–Cl bonds:*



Step 2. *We assign lone pairs of electrons to their atoms*. Each Cl atom now has seven electrons assigned to it, and the I atom has eight.

Step 3. *Subtract this number from the number of valence electrons for the neutral atom:*

I: 7 – 8 = –1
Cl: 7 – 7 = 0

The sum of the formal charges of all the atoms equals –1, which is identical to the charge of the ion (–1).

Exercise 4.2.1

Calculate the formal charge for each atom in the carbon monoxide molecule:



Answer

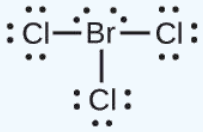
C −1, O +1

Example 4.2.2: Calculating Formal Charge from Lewis Structures

Assign formal charges to each atom in the interhalogen molecule $BrCl_3$.

Solution

Step 1. *Assign one of the electrons in each Br–Cl bond to the Br atom and one to the Cl atom in that bond:*



Step 2. *Assign the lone pairs to their atom.* Now each Cl atom has seven electrons and the Br atom has seven electrons.

Step 3. *Subtract this number from the number of valence electrons for the neutral atom.* This gives the formal charge:

Br: 7 – 7 = 0
Cl: 7 – 7 = 0

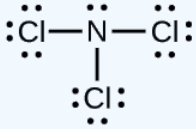
All atoms in $BrCl_3$ have a formal charge of zero, and the sum of the formal charges totals zero, as it must in a neutral molecule.

Exercise 4.2.2

Determine the formal charge for each atom in NCl_3.

Answer

N: 0; all three Cl atoms: 0

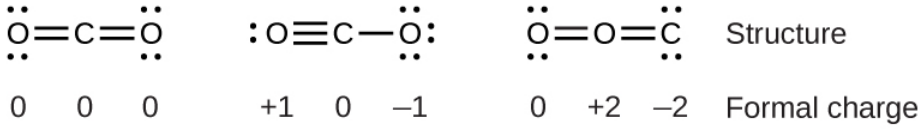


4.2.2: Using Formal Charge to Predict Molecular Structure

The arrangement of atoms in a molecule or ion is called its **molecular structure**. In many cases, following the steps for writing Lewis structures may lead to more than one possible molecular structure—different multiple bond and lone-pair electron placements or different arrangements of atoms, for instance. A few guidelines involving formal charge can be helpful in deciding which of the possible structures is most likely for a particular molecule or ion:

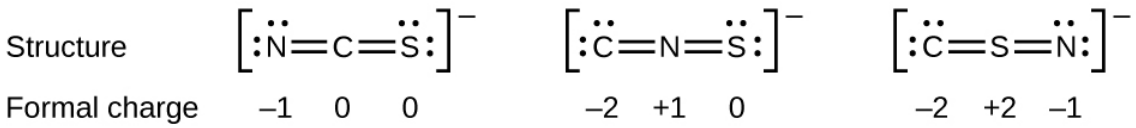
1. A molecular structure in which all formal charges are zero is preferable to one in which some formal charges are not zero.
2. If the Lewis structure must have nonzero formal charges, the arrangement with the smallest nonzero formal charges is preferable.
3. Lewis structures are preferable when adjacent formal charges are zero or of the opposite sign.
4. When we must choose among several Lewis structures with similar distributions of formal charges, the structure with the negative formal charges on the more electronegative atoms is preferable.

To see how these guidelines apply, let us consider some possible structures for carbon dioxide, CO_2. We know from our previous discussion that the less electronegative atom typically occupies the central position, but formal charges allow us to understand *why* this occurs. We can draw three possibilities for the structure: carbon in the center and double bonds, carbon in the center with a single and triple bond, and oxygen in the center with double bonds:



Comparing the three formal charges, we can definitively identify the structure on the left as preferable because it has only formal charges of zero (Guideline 1).

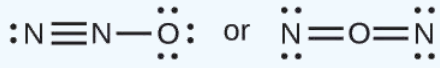
As another example, the thiocyanate ion, an ion formed from a carbon atom, a nitrogen atom, and a sulfur atom, could have three different molecular structures: NCS^-, CNS^-, or CSN^-. The formal charges present in each of these molecular structures can help us pick the most likely arrangement of atoms. Possible Lewis structures and the formal charges for each of the three possible structures for the thiocyanate ion are shown here:



Note that the sum of the formal charges in each case is equal to the charge of the ion (–1). However, the first arrangement of atoms is preferred because it has the lowest number of atoms with nonzero formal charges (Guideline 2). Also, it places the least electronegative atom in the center, and the negative charge on the more electronegative element (Guideline 4).

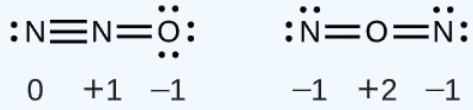
✔ Example 4.2.3: Using Formal Charge to Determine Molecular Structure

Nitrous oxide, N_2O, commonly known as laughing gas, is used as an anesthetic in minor surgeries, such as the routine extraction of wisdom teeth. Which is the more likely structure for nitrous oxide?

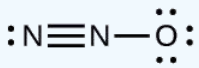


Solution

Determining formal charge yields the following:



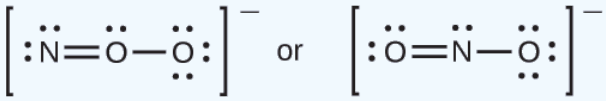
The structure with a terminal oxygen atom best satisfies the criteria for the most stable distribution of formal charge:



The number of atoms with formal charges are minimized (Guideline 2), there is no formal charge with a magnitude greater than one (Guideline 2), the negative formal charge is on the more electronegative element (Guideline 4), and the less electronegative atom is in the center position.

? Exercise 4.2.3

Which is the most likely molecular structure for the nitrite ion?



Answer

ONO^-

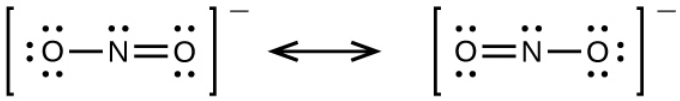
4.2.3: Resonance

Notice that the more likely structure for the nitrite anion in Example **4.2.3** may actually be drawn in two different ways, distinguished by the locations of the N-O and N=O bonds:



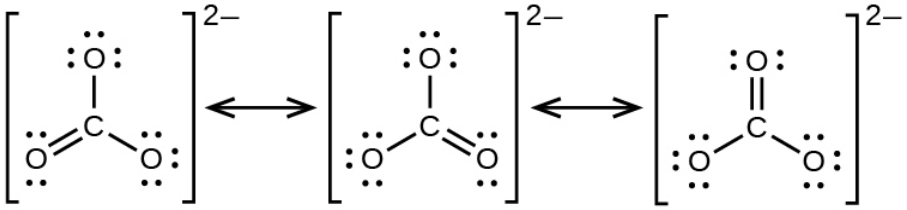
If nitrite ions do indeed contain a single and a double bond, we would expect for the two bond lengths to be different. A double bond between two atoms is shorter (and stronger) than a single bond between the same two atoms. Experiments show, however, that both N–O bonds in have the same strength and length, and are identical in all other properties.

It is not possible to write a single Lewis structure for in which nitrogen has an octet and both bonds are equivalent. Instead, we use the concept of **resonance**: if two or more Lewis structures with the same arrangement of atoms can be written for a molecule or ion, the actual distribution of electrons is an *average* of that shown by the various Lewis structures. The actual distribution of electrons in each of the nitrogen-oxygen bonds in is the average of a double bond and a single bond. We call the individual Lewis structures **resonance forms**. The actual electronic structure of the molecule (the average of the resonance forms) is called a **resonance hybrid** of the individual resonance forms. A double-headed arrow between Lewis structures indicates that they are resonance forms.



We should remember that a molecule described as a resonance hybrid *never* possesses an electronic structure described by either resonance form. It does not fluctuate between resonance forms; rather, the actual electronic structure is *always* the average of that shown by all resonance forms. George Wheland, one of the pioneers of resonance theory, used a historical analogy to describe the relationship between resonance forms and resonance hybrids. A medieval traveler, having never before seen a rhinoceros, described it as a hybrid of a dragon and a unicorn because it had many properties in common with both. Just as a rhinoceros is neither a dragon sometimes nor a unicorn at other times, a resonance hybrid is neither of its resonance forms at any given time. Like a rhinoceros, it is a real entity that experimental evidence has shown to exist. It has some characteristics in common with its resonance forms, but the resonance forms themselves are convenient, imaginary images (like the unicorn and the dragon).

The carbonate anion, provides a second example of resonance:



One oxygen atom must have a double bond to carbon to complete the octet on the central atom. All oxygen atoms, however, are equivalent, and the double bond could form from any one of the three atoms. This gives rise to three resonance forms of the carbonate ion. Because we can write three identical resonance structures, we know that the actual arrangement of electrons in the carbonate ion is the average of the three structures. Again, experiments show that all three C–O bonds are exactly the same.

Link to Learning

Use this online quiz to practice your skills in drawing resonance structures and estimating formal charges.

This page titled 4.2: Formal Charges and Resonance is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **7.4: Formal Charges and Resonance** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

4.3: Molecular Structure and Polarity

Learning Objectives

By the end of this section, you will be able to:

- Predict the structures of small molecules using valence shell electron pair repulsion (VSEPR) theory
- Explain the concepts of polar covalent bonds and molecular polarity
- Assess the polarity of a molecule based on its bonding and structure

Thus far, we have used two-dimensional Lewis structures to represent molecules. However, molecular structure is actually three-dimensional, and it is important to be able to describe molecular bonds in terms of their distances, angles, and relative arrangements in space (Figure **4.3.1**). A bond angle is the angle between any two bonds that include a common atom, usually measured in degrees. A bond distance (or bond length) is the distance between the nuclei of two bonded atoms along the straight line joining the nuclei. Bond distances are measured in Ångstroms (1 Å = 10^{-10} m) or picometers (1 pm = 10^{-12} m, 100 pm = 1 Å).

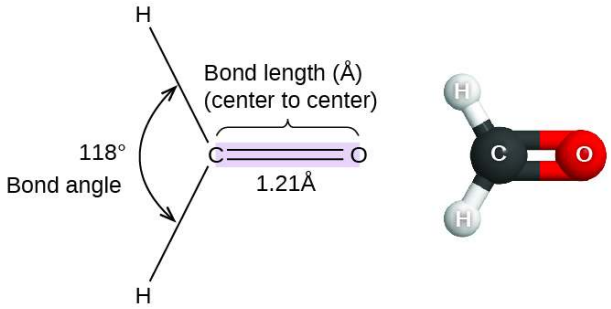


Figure **4.3.1**: Bond distances (lengths) and angles are shown for the formaldehyde molecule, H_2CO.

4.3.1: VSEPR Theory

Valence shell electron-pair repulsion theory (VSEPR theory) enables us to predict the molecular structure, including approximate bond angles around a central atom, of a molecule from an examination of the number of bonds and lone electron pairs in its Lewis structure. The VSEPR model assumes that electron pairs in the valence shell of a central atom will adopt an arrangement that minimizes repulsions between these electron pairs by maximizing the distance between them. The electrons in the valence shell of a central atom form either bonding pairs of electrons, located primarily between bonded atoms, or lone pairs. The electrostatic repulsion of these electrons is reduced when the various regions of high electron density assume positions as far from each other as possible.

VSEPR theory predicts the arrangement of electron pairs around each central atom and, usually, the correct arrangement of atoms in a molecule. We should understand, however, that the theory only considers electron-pair repulsions. Other interactions, such as nuclear-nuclear repulsions and nuclear-electron attractions, are also involved in the final arrangement that atoms adopt in a particular molecular structure.

As a simple example of VSEPR theory, let us predict the structure of a gaseous BeF_2 molecule. The Lewis structure of BeF_2 (Figure **4.3.2**) shows only two electron pairs around the central beryllium atom. With two bonds and no lone pairs of electrons on the central atom, the bonds are as far apart as possible, and the electrostatic repulsion between these regions of high electron density is reduced to a minimum when they are on opposite sides of the central atom. The bond angle is 180° (Figure **4.3.2**).

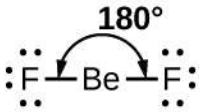


Figure **4.3.2**: The BeF_2 molecule adopts a linear structure in which the two bonds are as far apart as possible, on opposite sides of the Be atom.

Figure **4.3.3** illustrates this and other electron-pair geometries that minimize the repulsions among regions of high electron density (bonds and/or lone pairs). Two regions of electron density around a central atom in a molecule form a linear geometry; three

regions form a trigonal planar geometry; four regions form a tetrahedral geometry; five regions form a trigonal bipyramidal geometry; and six regions form an octahedral geometry.

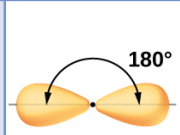
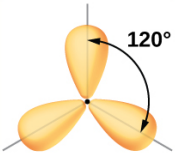
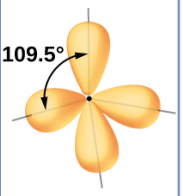
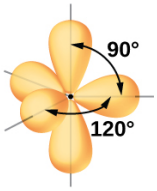
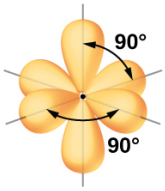
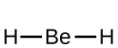
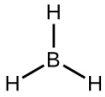
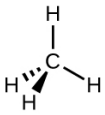
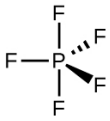
Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)	Five regions of high electron density (bonds and/or unshared pairs)	Six regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement					
Line-dash-wedge notation					
Electron region geometry	Linear; 180° angle	Trigonal planar; all angles 120°	Tetrahedral; all angles 109.5°	Trigonal bipyramidal; angles of 90° or 120° An attached atom may be equatorial (in the plane of the triangle) or axial (above or below the plane of the triangle).	Octahedral; all angles 90° or 180°

Figure **4.3.3**: The basic electron-pair geometries predicted by VSEPR theory maximize the space around any region of electron density (bonds or lone pairs).

4.3.1.1: Electron-pair Geometry versus Molecular Structure

It is important to note that electron-pair geometry around a central atom is *not* the same thing as its molecular structure. The electron-pair geometries shown in Figure **4.3.3** describe all regions where electrons are located, bonds as well as lone pairs. Molecular structure describes the location of the *atoms*, not the electrons.

We differentiate between these two situations by naming the geometry that includes *all* electron pairs the electron-pair geometry. The structure that includes only the placement of the atoms in the molecule is called the molecular structure. The electron-pair geometries will be the same as the molecular structures when there are no lone electron pairs around the central atom, but they will be different when there are lone pairs present on the central atom.

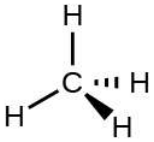


Figure **4.3.4**: The molecular structure of the methane molecule, CH_4, is shown with a tetrahedral arrangement of the hydrogen atoms. VSEPR structures like this one are often drawn using the wedge and dash notation, in which solid lines represent bonds in the plane of the page, solid wedges represent bonds coming up out of the plane, and dashed lines represent bonds going down into the plane.

For example, the methane molecule, CH_4, which is the major component of natural gas, has four bonding pairs of electrons around the central carbon atom; the electron-pair geometry is tetrahedral, as is the molecular structure (Figure **4.3.4**). On the other hand, the ammonia molecule, NH_3, also has four electron pairs associated with the nitrogen atom, and thus has a tetrahedral electron-pair geometry. One of these regions, however, is a lone pair, which is not included in the molecular structure, and this lone pair influences the shape of the molecule (Figure **4.3.5**).

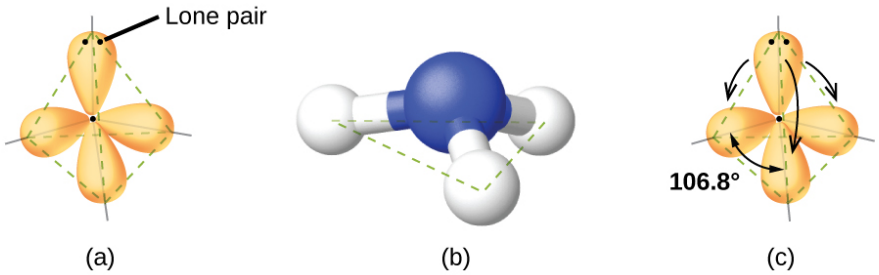


Figure **4.3.5**: (a) The electron-pair geometry for the ammonia molecule is tetrahedral with one lone pair and three single bonds. (b) The trigonal pyramidal molecular structure is determined from the electron-pair geometry. (c) The actual bond angles deviate slightly from the idealized angles because the lone pair takes up a larger region of space than do the single bonds, causing the HNH angle to be slightly smaller than 109.5°.

As seen in Figure **4.3.5**, small distortions from the ideal angles in Figure **4.3.3** can result from differences in repulsion between various regions of electron density. VSEPR theory predicts these distortions by establishing an order of repulsions and an order of the amount of space occupied by different kinds of electron pairs. The order of electron-pair repulsions from greatest to least repulsion is:

$$\text{lone pair-lone pair} > \text{lone pair-bonding pair} > \text{bonding pair-bonding pair}$$

This order of repulsions determines the amount of space occupied by different regions of electrons. A lone pair of electrons occupies a larger region of space than the electrons in a triple bond; in turn, electrons in a triple bond occupy more space than those in a double bond, and so on. The order of sizes from largest to smallest is:

$$\text{lone pair} > \text{triple bond} > \text{double bond} > \text{single bond}$$

Consider formaldehyde, H_2CO, which is used as a preservative for biological and anatomical specimens (Figure **4.3.1**). This molecule has regions of high electron density that consist of two single bonds and one double bond. The basic geometry is trigonal planar with 120° bond angles, but we see that the double bond causes slightly larger angles (121°), and the angle between the single bonds is slightly smaller (118°).

In the ammonia molecule, the three hydrogen atoms attached to the central nitrogen are not arranged in a flat, trigonal planar molecular structure, but rather in a three-dimensional trigonal pyramid (Figure **4.3.5**) with the nitrogen atom at the apex and the three hydrogen atoms forming the base. The ideal bond angles in a trigonal pyramid are based on the tetrahedral electron pair geometry. Again, there are slight deviations from the ideal because lone pairs occupy larger regions of space than do bonding electrons. The H–N–H bond angles in NH_3 are slightly smaller than the 109.5° angle in a regular tetrahedron (Figure **4.3.3**) because the lone pair-bonding pair repulsion is greater than the bonding pair-bonding pair repulsion (Figure **4.3.5**). Figure **4.3.6** illustrates the ideal molecular structures, which are predicted based on the electron-pair geometries for various combinations of lone pairs and bonding pairs.

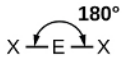
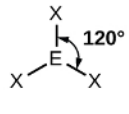
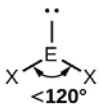
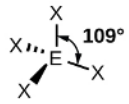
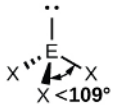
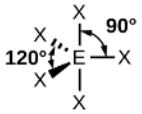
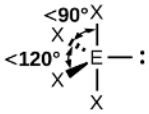
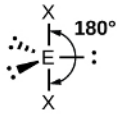
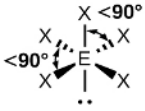
Number of electron regions	Electron region geometries: 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal planar	 Bent or angular			
4	 Tetrahedral	 Trigonal pyramid	 Bent or angular		
5	 Trigonal bipyramid	 Sawhorse or seesaw	 T-shape	 Linear	
6	 Octahedral	 Square pyramid	 Square planar	 T-shape	 Linear

Figure **4.3.6**: The molecular structures are identical to the electron-pair geometries when there are no lone pairs present (first column). For a particular number of electron pairs (row), the molecular structures for one or more lone pairs are determined based on modifications of the corresponding electron-pair geometry.

According to VSEPR theory, the terminal atom locations (Xs in Figure **4.3.6**) are equivalent within the linear, trigonal planar, and tetrahedral electron-pair geometries (the first three rows of the table). It does not matter which X is replaced with a lone pair because the molecules can be rotated to convert positions. For trigonal bipyramidal electron-pair geometries, however, there are two distinct X positions, as shown in Figure **4.3.7** an axial position (if we hold a model of a trigonal bipyramid by the two axial positions, we have an axis around which we can rotate the model) and an equatorial position (three positions form an equator around the middle of the molecule). As shown in Figure **4.3.6**, the axial position is surrounded by bond angles of 90°, whereas the equatorial position has more space available because of the 120° bond angles. In a trigonal bipyramidal electron-pair geometry, lone pairs always occupy equatorial positions because these more spacious positions can more easily accommodate the larger lone pairs.

Theoretically, we can come up with three possible arrangements for the three bonds and two lone pairs for the ClF_3 molecule (Figure **4.3.7**). The stable structure is the one that puts the lone pairs in equatorial locations, giving a T-shaped molecular structure.

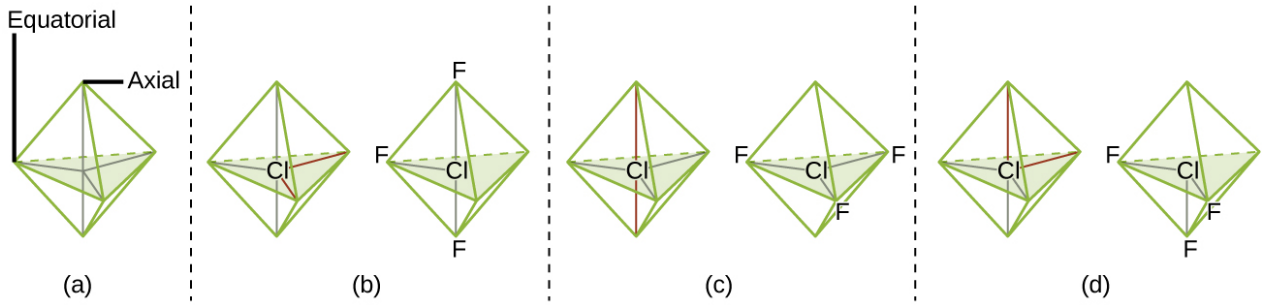


Figure **4.3.7**: (a) In a trigonal bipyramid, the two axial positions are located directly across from one another, whereas the three equatorial positions are located in a triangular arrangement. (b–d) The two lone pairs (red lines) in ClF_3 have several possible arrangements, but the T-shaped molecular structure (b) is the one actually observed, consistent with the larger lone pairs both occupying equatorial positions.

When a central atom has two lone electron pairs and four bonding regions, we have an octahedral electron-pair geometry. The two lone pairs are on opposite sides of the octahedron (180° apart), giving a square planar molecular structure that minimizes lone pair-lone pair repulsions (Figure **4.3.6**).

4.3.1.2: Predicting Electron Pair Geometry and Molecular Structure

The following procedure uses VSEPR theory to determine the electron pair geometries and the molecular structures:

1. Write the Lewis structure of the molecule or polyatomic ion.
2. Count the number of regions of electron density (lone pairs and bonds) around the central atom. A single, double, or triple bond counts as one region of electron density.
3. Identify the electron-pair geometry based on the number of regions of electron density: linear, trigonal planar, tetrahedral, trigonal bipyramidal, or octahedral (Figure **4.3.6**, first column).
4. Use the number of lone pairs to determine the molecular structure (Figure **4.3.6**). If more than one arrangement of lone pairs and chemical bonds is possible, choose the one that will minimize repulsions, remembering that lone pairs occupy more space than multiple bonds, which occupy more space than single bonds. In trigonal bipyramidal arrangements, repulsion is minimized when every lone pair is in an equatorial position. In an octahedral arrangement with two lone pairs, repulsion is minimized when the lone pairs are on opposite sides of the central atom.

The following examples illustrate the use of VSEPR theory to predict the molecular structure of molecules or ions that have no lone pairs of electrons. In this case, the molecular structure is identical to the electron pair geometry.

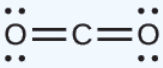
✔ Example **4.3.1**: Predicting Electron-pair Geometry and Molecular Structure: CO_2 and BCl_3

Predict the electron-pair geometry and molecular structure for each of the following:

a. carbon dioxide, CO_2, a molecule produced by the combustion of fossil fuels
b. boron trichloride, BCl_3, an important industrial chemical

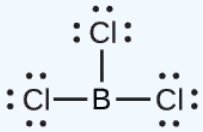
Solution

(a) We write the Lewis structure of CO_2 as:



This shows us two regions of high electron density around the carbon atom—each double bond counts as one region, and there are no lone pairs on the carbon atom. Using VSEPR theory, we predict that the two regions of electron density arrange themselves on opposite sides of the central atom with a bond angle of 180°. The electron-pair geometry and molecular structure are identical, and CO_2 molecules are linear.

(b) We write the Lewis structure of BCl_3 as:



Thus we see that BCl_3 contains three bonds, and there are no lone pairs of electrons on boron. The arrangement of three regions of high electron density gives a trigonal planar electron-pair geometry. The B–Cl bonds lie in a plane with 120° angles between them. BCl_3 also has a trigonal planar molecular structure (Figure **4.3.8**).

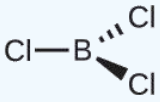


Figure **4.3.8**:

The electron-pair geometry and molecular structure of BCl_3 are both trigonal planar. Note that the VSEPR geometry indicates the correct bond angles (120°), unlike the Lewis structure shown above.

? Exercise 4.3.1

Carbonate, is a common polyatomic ion found in various materials from eggshells to antacids. What are the electron-pair geometry and molecular structure of this polyatomic ion?

Answer

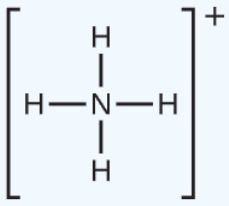
The electron-pair geometry is trigonal planar and the molecular structure is trigonal planar. Due to resonance, all three C–O bonds are identical. Whether they are single, double, or an average of the two, each bond counts as one region of electron density.

✓ Example 4.3.2: Predicting Electron-pair Geometry and Molecular Structure: Ammonium

Two of the top 50 chemicals produced in the United States, ammonium nitrate and ammonium sulfate, both used as fertilizers, contain the ammonium ion. Predict the electron-pair geometry and molecular structure of the cation.

Solution

We write the Lewis structure of as:



We can see that NH_4^+ contains four bonds from the nitrogen atom to hydrogen atoms and no lone pairs. We expect the four regions of high electron density to arrange themselves so that they point to the corners of a tetrahedron with the central nitrogen atom in the middle (Figure **4.3.6**). Therefore, the electron pair geometry of Figure **4.3.9**.

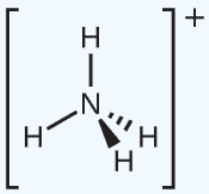


Figure **4.3.9**: The ammonium ion displays a tetrahedral electron-pair geometry as well as a tetrahedral molecular structure.

Exercise 4.3.2

Identify a molecule with trigonal bipyramidal molecular structure.

Answer

Any molecule with five electron pairs around the central atoms including no lone pairs will be trigonal bipyramidal. PF_5 is a common example.

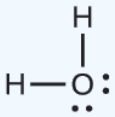
The next several examples illustrate the effect of lone pairs of electrons on molecular structure.

Example 4.3.3: Predicting Electron-pair Geometry and Molecular Structure: Lone Pairs on the Central Atom

Predict the electron-pair geometry and molecular structure of a water molecule.

Solution

The Lewis structure of H_2O indicates that there are four regions of high electron density around the oxygen atom: two lone pairs and two chemical bonds:



We predict that these four regions are arranged in a tetrahedral fashion (Figure 4.3.10), as indicated in Figure 4.3.6. Thus, the electron-pair geometry is tetrahedral and the molecular structure is bent with an angle slightly less than 109.5°. In fact, the bond angle is 104.5°.

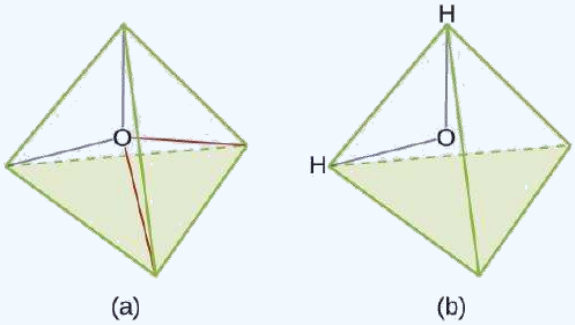


Figure 4.3.10: (a) H_2O has four regions of electron density around the central atom, so it has a tetrahedral electron-pair geometry. (b) Two of the electron regions are lone pairs, so the molecular structure is bent.

Exercise 4.3.3

The hydronium ion, H_3O^+, forms when acids are dissolved in water. Predict the electron-pair geometry and molecular structure of this cation.

Answer

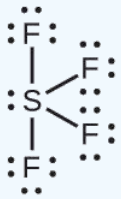
electron pair geometry: tetrahedral; molecular structure: trigonal pyramidal

Example 4.3.4: Predicting Electron-pair Geometry and Molecular Structure: SF_4

Sulfur tetrafluoride, SF_4, is extremely valuable for the preparation of fluorine-containing compounds used as herbicides (i.e., SF_4 is used as a fluorinating agent). Predict the electron-pair geometry and molecular structure of a SF_4 molecule.

Solution

The Lewis structure of SF_4 indicates five regions of electron density around the sulfur atom: one lone pair and four bonding pairs:



We expect these five regions to adopt a trigonal bipyramidal electron-pair geometry. To minimize lone pair repulsions, the lone pair occupies one of the equatorial positions. The molecular structure (Figure **4.3.11**) is that of a seesaw (Figure **4.3.6**).

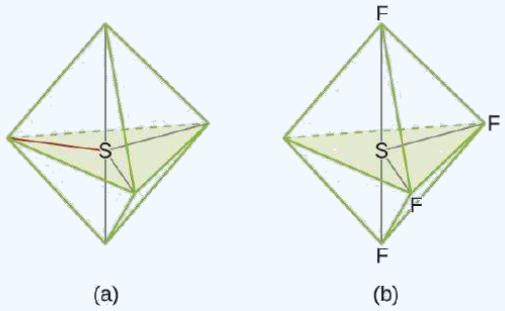


Figure **4.3.11**: (a) SF4 has a trigonal bipyramidal arrangement of the five regions of electron density. (b) One of the regions is a lone pair, which results in a seesaw-shaped molecular structure.

Exercise 4.3.4

Predict the electron pair geometry and molecular structure for molecules of XeF_2.

Answer

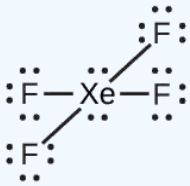
The electron-pair geometry is trigonal bipyramidal. The molecular structure is linear.

Example 4.3.5: Predicting Electron-pair Geometry and Molecular Structure: XeF_4

Of all the noble gases, xenon is the most reactive, frequently reacting with elements such as oxygen and fluorine. Predict the electron-pair geometry and molecular structure of the XeF_4 molecule.

Solution

The Lewis structure of XeF_4 indicates six regions of high electron density around the xenon atom: two lone pairs and four bonds:



These six regions adopt an octahedral arrangement (Figure **4.3.6**), which is the electron-pair geometry. To minimize repulsions, the lone pairs should be on opposite sides of the central atom (Figure **4.3.12**). The five atoms are all in the same plane and have a square planar molecular structure.

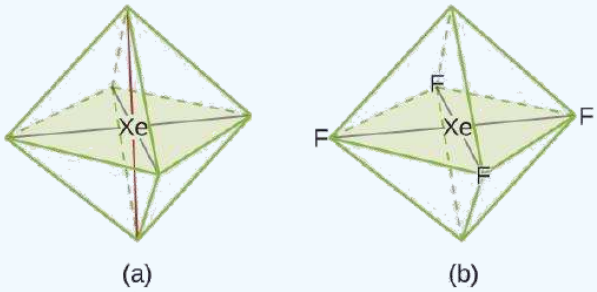


Figure **4.3.12**: (a) XeF_4 adopts an octahedral arrangement with two lone pairs (red lines) and four bonds in the electron-pair geometry. (b) The molecular structure is square planar with the lone pairs directly across from one another.

? Exercise 4.3.5

In a certain molecule, the central atom has three lone pairs and two bonds. What will the electron pair geometry and molecular structure be?

Answer

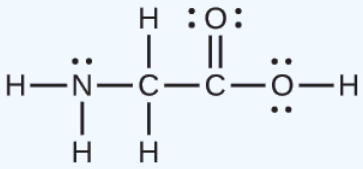
electron pair geometry: trigonal bipyramidal; molecular structure: linear

4.3.1.3: Molecular Structure for Multicenter Molecules

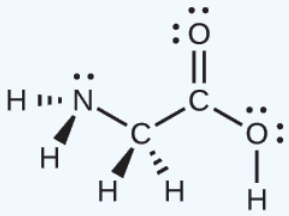
When a molecule or polyatomic ion has only one central atom, the molecular structure completely describes the shape of the molecule. Larger molecules do not have a single central atom, but are connected by a chain of interior atoms that each possess a "local" geometry. The way these local structures are oriented with respect to each other also influences the molecular shape, but such considerations are largely beyond the scope of this introductory discussion. For our purposes, we will only focus on determining the local structures.

✓ Example 4.3.6: Predicting Structure in Multicenter Molecules

The Lewis structure for the simplest amino acid, glycine, $H_2NCH_2CO_2H$, is shown here. Predict the local geometry for the nitrogen atom, the two carbon atoms, and the oxygen atom with a hydrogen atom attached:



Solution



Consider each central atom independently. The electron-pair geometries:

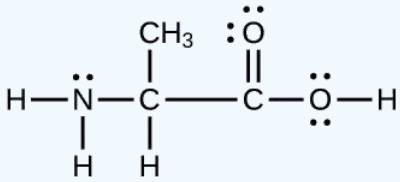
- nitrogen—four regions of electron density; tetrahedral
- carbon ($\underline{C}H_2$)—four regions of electron density; tetrahedral
- carbon ($\underline{C}O_2$)—three regions of electron density; trigonal planar
- oxygen ($\underline{O}H$)—four regions of electron density; tetrahedral

The local structures:

- nitrogen—three bonds, one lone pair; trigonal pyramidal
- carbon ($\underline{C}H_2$)—four bonds, no lone pairs; tetrahedral
- carbon ($\underline{C}O_2$)—three bonds (double bond counts as one bond), no lone pairs; trigonal planar
- oxygen ($\underline{O}H$)—two bonds, two lone pairs; bent (109°)

Exercise 4.3.6

Another amino acid is alanine, which has the Lewis structure shown here. Predict the electron-pair geometry and local structure of the nitrogen atom, the three carbon atoms, and the oxygen atom with hydrogen attached:



Answer

electron-pair geometries: nitrogen—tetrahedral; carbon ($\underline{C}H$)—tetrahedral; carbon ($\underline{C}H_3$)—tetrahedral; carbon ($\underline{C}O_2$)—trigonal planar; oxygen ($\underline{O}H$)—tetrahedral; local structures: nitrogen—trigonal pyramidal; carbon ($\underline{C}H$)—tetrahedral; carbon ($\underline{C}H_3$)—tetrahedral; carbon ($\underline{C}O_2$)—trigonal planar; oxygen ($\underline{O}H$)—bent (109°)

Link to Learning

The molecular shape simulator lets you build various molecules and practice naming their electron-pair geometries and molecular structures.

Example 4.3.7: Molecular Simulation

Using molecular shape simulator allows us to control whether bond angles and/or lone pairs are displayed by checking or unchecking the boxes under “Options” on the right. We can also use the “Name” checkboxes at bottom-left to display or hide the electron pair geometry (called “electron geometry” in the simulator) and/or molecular structure (called “molecular shape” in the simulator).

Build the molecule HCN in the simulator based on the following Lewis structure:

$$\mathbf{H{-}C{\equiv}N}$$

Click on each bond type or lone pair at right to add that group to the central atom. Once you have the complete molecule, rotate it to examine the predicted molecular structure. What molecular structure is this?

Solution

The molecular structure is linear.

Exercise 4.3.7

Build a more complex molecule in the simulator. Identify the electron-group geometry, molecular structure, and bond angles. Then try to find a chemical formula that would match the structure you have drawn.

Answer

Answers will vary. For example, an atom with four single bonds, a double bond, and a lone pair has an octahedral electron-group geometry and a square pyramidal molecular structure. $XeOF_4$ is a molecule that adopts this structure.

4.3.2: Molecular Polarity and Dipole Moment

As discussed previously, polar covalent bonds connect two atoms with differing electronegativities, leaving one atom with a partial positive charge (δ+) and the other atom with a partial negative charge (δ–), as the electrons are pulled toward the more electronegative atom. This separation of charge gives rise to a bond dipole moment. The magnitude of a bond dipole moment is represented by the Greek letter mu (μ) and is given by the formula shown here, where Q is the magnitude of the partial charges (determined by the electronegativity difference) and r is the distance between the charges:

$$\mu = Qr$$

This bond moment can be represented as a vector, a quantity having both direction and magnitude (Figure **4.3.13**). Dipole vectors are shown as arrows pointing along the bond from the less electronegative atom toward the more electronegative atom. A small plus sign is drawn on the less electronegative end to indicate the partially positive end of the bond. The length of the arrow is proportional to the magnitude of the electronegativity difference between the two atoms.

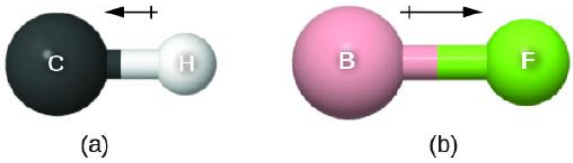


Figure **4.3.13**: (a) There is a small difference in electronegativity between C and H, represented as a short vector. (b) The electronegativity difference between B and F is much larger, so the vector representing the bond moment is much longer.

A whole molecule may also have a separation of charge, depending on its molecular structure and the polarity of each of its bonds. If such a charge separation exists, the molecule is said to be a polar molecule (or dipole); otherwise the molecule is said to be nonpolar. The dipole moment measures the extent of net charge separation in the molecule as a whole. We determine the dipole moment by adding the bond moments in three-dimensional space, taking into account the molecular structure.

For diatomic molecules, there is only one bond, so its bond dipole moment determines the molecular polarity. Homonuclear diatomic molecules such as Br_2 and N_2 have no difference in electronegativity, so their dipole moment is zero. For heteronuclear molecules such as CO, there is a small dipole moment. For HF, there is a larger dipole moment because there is a larger difference in electronegativity.

When a molecule contains more than one bond, the geometry must be taken into account. If the bonds in a molecule are arranged such that their bond moments cancel (vector sum equals zero), then the molecule is nonpolar. This is the situation in CO_2 (Figure **4.3.14**). Each of the bonds is polar, but the molecule as a whole is nonpolar. From the Lewis structure, and using VSEPR theory, we determine that the CO_2 molecule is linear with polar C=O bonds on opposite sides of the carbon atom. The bond moments cancel because they are pointed in opposite directions. In the case of the water molecule (Figure **4.3.14**), the Lewis structure again shows that there are two bonds to a central atom, and the electronegativity difference again shows that each of these bonds has a nonzero bond moment. In this case, however, the molecular structure is bent because of the lone pairs on O, and the two bond moments do not cancel. Therefore, water does have a net dipole moment and is a polar molecule (dipole).

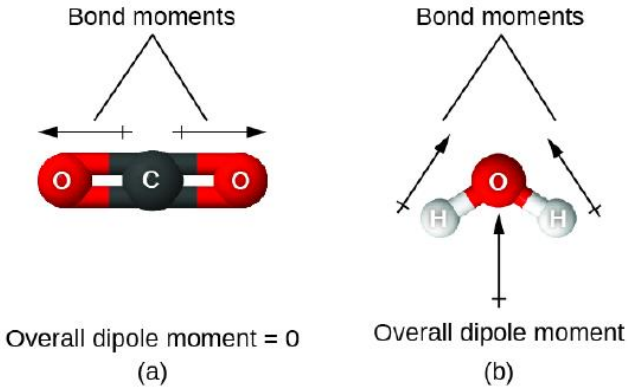
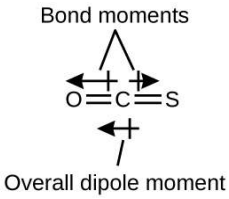


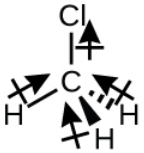
Figure **4.3.14**: The overall dipole moment of a molecule depends on the individual bond dipole moments and how they are arranged. (a) Each CO bond has a bond dipole moment, but they point in opposite directions so that the net CO_2 molecule is nonpolar. (b) In contrast, water is polar because the OH bond moments do not cancel out.

The OCS molecule has a structure similar to CO_2, but a sulfur atom has replaced one of the oxygen atoms. To determine if this molecule is polar, we draw the molecular structure. VSEPR theory predicts a linear molecule:

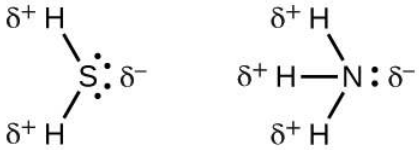


The C-O bond is considerably polar. Although C and S have very similar electronegativity values, S is slightly more electronegative than C, and so the C-S bond is just slightly polar. Because oxygen is more electronegative than sulfur, the oxygen end of the molecule is the negative end.

Chloromethane, CH_3Cl, is a tetrahedral molecule with three slightly polar C-H bonds and a more polar C-Cl bond. The relative electronegativities of the bonded atoms is H < C < Cl, and so the bond moments all point toward the Cl end of the molecule and sum to yield a considerable dipole moment (the molecules are relatively polar).



For molecules of high symmetry such as BF_3 (trigonal planar), CH_4 (tetrahedral), PF_5 (trigonal bipyramidal), and SF_6 (octahedral), all the bonds are of identical polarity (same bond moment) and they are oriented in geometries that yield nonpolar molecules (dipole moment is zero). Molecules of less geometric symmetry, however, may be polar even when all bond moments are identical. For these molecules, the directions of the equal bond moments are such that they sum to give a nonzero dipole moment and a polar molecule. Examples of such molecules include hydrogen sulfide, H_2S (nonlinear), and ammonia, NH_3 (trigonal pyramidal).



To summarize, to be polar, a molecule must:

1. Contain at least one polar covalent bond.
2. Have a molecular structure such that the sum of the vectors of each bond dipole moment does not cancel.

4.3.2.1: Properties of Polar Molecules

Polar molecules tend to align when placed in an electric field with the positive end of the molecule oriented toward the negative plate and the negative end toward the positive plate (Figure **4.3.15**). We can use an electrically charged object to attract polar molecules, but nonpolar molecules are not attracted. Also, polar solvents are better at dissolving polar substances, and nonpolar solvents are better at dissolving nonpolar substances.

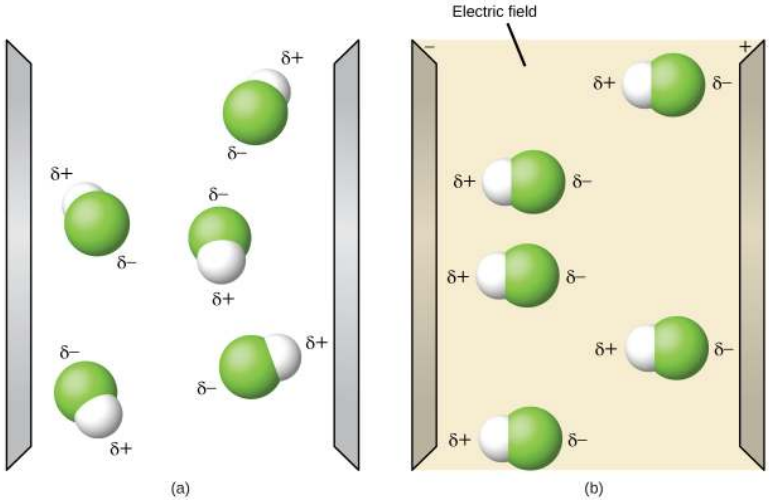


Figure **4.3.15**: (a) Molecules are always randomly distributed in the liquid state in the absence of an electric field. (b) When an electric field is applied, polar molecules like HF will align to the dipoles with the field direction.

Link to Learning

The molecule polarity simulation provides many ways to explore dipole moments of bonds and molecules.

Example 4.3.8: Polarity Simulations

Open the molecule polarity simulation and select the "Three Atoms" tab at the top. This should display a molecule ABC with three electronegativity adjustors. You can display or hide the bond moments, molecular dipoles, and partial charges at the right. Turning on the Electric Field will show whether the molecule moves when exposed to a field, similar to Figure **4.3.15**.

Use the electronegativity controls to determine how the molecular dipole will look for the starting bent molecule if:

a. A and C are very electronegative and B is in the middle of the range.
b. A is very electronegative, and B and C are not.

Solution

a. Molecular dipole moment points immediately between A and C.
b. Molecular dipole moment points along the A–B bond, toward A.

Exercise 4.3.8

Determine the partial charges that will give the largest possible bond dipoles.

Answer

The largest bond moments will occur with the largest partial charges. The two solutions above represent how unevenly the electrons are shared in the bond. The bond moments will be maximized when the electronegativity difference is greatest. The controls for A and C should be set to one extreme, and B should be set to the opposite extreme. Although the magnitude of the bond moment will not change based on whether B is the most electronegative or the least, the direction of the bond moment will.

This page titled 4.3: Molecular Structure and Polarity is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **7.6: Molecular Structure and Polarity** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

4.4: Valence Bond Theory

Learning Objectives

By the end of this section, you will be able to:

- Describe the formation of covalent bonds in terms of atomic orbital overlap
- Define and give examples of σ and π bonds

As we know, a scientific theory is a strongly supported explanation for observed natural laws or large bodies of experimental data. For a theory to be accepted, it must explain experimental data and be able to predict behavior. For example, VSEPR theory has gained widespread acceptance because it predicts three-dimensional molecular shapes that are consistent with experimental data collected for thousands of different molecules. However, VSEPR theory does not provide an explanation of chemical bonding.

There are successful theories that describe the electronic structure of atoms. We can use quantum mechanics to predict the specific regions around an atom where electrons are likely to be located: A spherical shape for an *s* orbital, a dumbbell shape for a *p* orbital, and so forth. However, these predictions only describe the orbitals around free atoms. When atoms bond to form molecules, atomic orbitals are not sufficient to describe the regions where electrons will be located in the molecule. A more complete understanding of electron distributions requires a model that can account for the electronic structure of molecules. One popular theory holds that a covalent bond forms when a pair of electrons is shared by two atoms and is simultaneously attracted by the nuclei of both atoms. In the following sections, we will discuss how such bonds are described by valence bond theory and hybridization.

Valence bond theory describes a covalent bond as the overlap of half-filled atomic orbitals (each containing a single electron) that yield a pair of electrons shared between the two bonded atoms. We say that orbitals on two different atoms overlap when a portion of one orbital and a portion of a second orbital occupy the same region of space. According to valence bond theory, a covalent bond results when two conditions are met: (1) an orbital on one atom overlaps an orbital on a second atom and (2) the single electrons in each orbital combine to form an electron pair. The mutual attraction between this negatively charged electron pair and the two atoms' positively charged nuclei serves to physically link the two atoms through a force we define as a covalent bond. The strength of a covalent bond depends on the extent of overlap of the orbitals involved. Orbitals that overlap extensively form bonds that are stronger than those that have less overlap.

The energy of the system depends on how much the orbitals overlap. Figure **4.4.1** illustrates how the sum of the energies of two hydrogen atoms (the colored curve) changes as they approach each other. When the atoms are far apart there is no overlap, and by convention we set the sum of the energies at zero. As the atoms move together, their orbitals begin to overlap. Each electron begins to feel the attraction of the nucleus in the other atom. In addition, the electrons begin to repel each other, as do the nuclei. While the atoms are still widely separated, the attractions are slightly stronger than the repulsions, and the energy of the system decreases. (A bond begins to form.) As the atoms move closer together, the overlap increases, so the attraction of the nuclei for the electrons continues to increase (as do the repulsions among electrons and between the nuclei). At some specific distance between the atoms, which varies depending on the atoms involved, the energy reaches its lowest (most stable) value. This optimum distance between the two bonded nuclei is the bond distance between the two atoms. The bond is stable because at this point, the attractive and repulsive forces combine to create the lowest possible energy configuration. If the distance between the nuclei were to decrease further, the repulsions between nuclei and the repulsions as electrons are confined in closer proximity to each other would become stronger than the attractive forces. The energy of the system would then rise (making the system destabilized), as shown at the far left of Figure **4.4.1**.

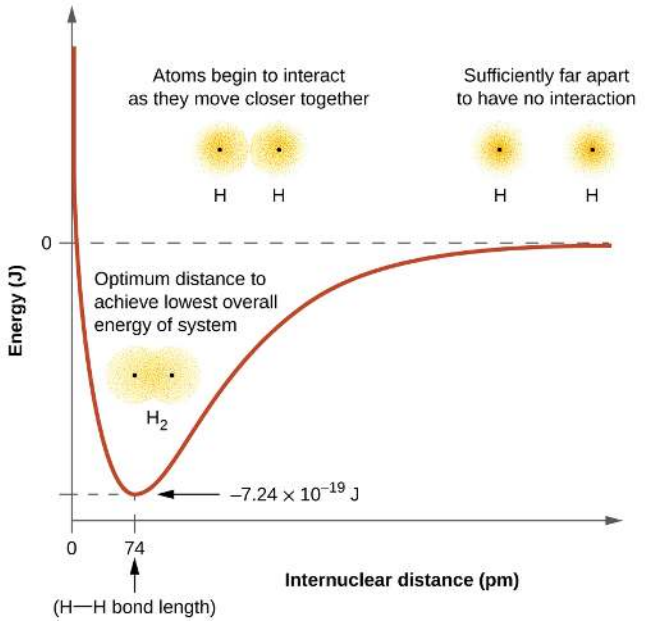


Figure **4.4.1**: (a) The interaction of two hydrogen atoms changes as a function of distance. (b) The energy of the system changes as the atoms interact. The lowest (most stable) energy occurs at a distance of 74 pm, which is the bond length observed for the H_2 molecule.

The bond energy is the difference between the energy minimum (which occurs at the bond distance) and the energy of the two separated atoms. This is the quantity of energy released when the bond is formed. Conversely, the same amount of energy is required to break the bond. For the H_2 molecule shown in Figure **4.4.1**, at the bond distance of 74 pm the system is $\mathbf{7.24 \times 10^{-19}\ J}$ lower in energy than the two separated hydrogen atoms. This may seem like a small number. However, we know from our earlier description of thermochemistry that bond energies are often discussed on a per-mole basis. For example, it requires $\mathbf{7.24 \times 10^{-19}\ J}$ to break one H–H bond, but it takes $\mathbf{4.36 \times 10^{5}\ J}$ to break 1 mole of H–H bonds. A comparison of some bond lengths and energies is shown in Table **4.4.1**. We can find many of these bonds in a variety of molecules, and this table provides average values. For example, breaking the first C–H bond in CH_4 requires 439.3 kJ/mol, while breaking the first C–H bond in $H–CH_2C_6H_5$ (a common paint thinner) requires 375.5 kJ/mol.

Table **4.4.1**: Representative Bond Energies and Lengths

Bond	Length (pm)	Energy (kJ/mol)	Bond	Length (pm)	Energy (kJ/mol)
H–H	74	436	C–O	140.1	358
H–C	106.8	413		119.7	745
H–N	101.5	391		113.7	1072
H–O	97.5	467	H–Cl	127.5	431
C–C	150.6	347	H–Br	141.4	366
	133.5	614	H–I	160.9	298
	120.8	839	O–O	148	146
C–N	142.1	305		120.8	498
	130.0	615	F–F	141.2	159
	116.1	891	Cl–Cl	198.8	243

In addition to the distance between two orbitals, the orientation of orbitals also affects their overlap (other than for two *s* orbitals, which are spherically symmetric). Greater overlap is possible when orbitals are oriented such that they overlap on a direct line

between the two nuclei. Figure **4.4.2** illustrates this for two *p* orbitals from different atoms; the overlap is greater when the orbitals overlap end to end rather than at an angle.

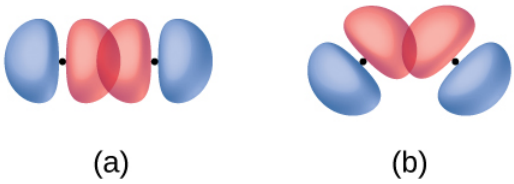


Figure **4.4.2**: (a) The overlap of two *p* orbitals is greatest when the orbitals are directed end to end. (b) Any other arrangement results in less overlap. The dots indicate the locations of the nuclei.

The overlap of two *s* orbitals (as in H_2), the overlap of an *s* orbital and a *p* orbital (as in HCl), and the end-to-end overlap of two *p* orbitals (as in Cl_2) all produce sigma bonds (σ bonds), as illustrated in Figure **4.4.3**. A σ bond is a covalent bond in which the electron density is concentrated in the region along the internuclear axis; that is, a line between the nuclei would pass through the center of the overlap region. Single bonds in Lewis structures are described as σ bonds in valence bond theory.

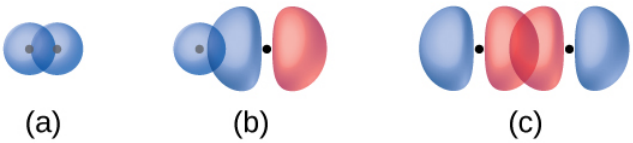


Figure **4.4.3**: Sigma (σ) bonds form from the overlap of the following: (a) two *s* orbitals, (b) an *s* orbital and a *p* orbital, and (c) two *p* orbitals. The dots indicate the locations of the nuclei.

A pi bond (π bond) is a type of covalent bond that results from the side-by-side overlap of two *p* orbitals, as illustrated in Figure **4.4.4**. In a π bond, the regions of orbital overlap lie on opposite sides of the internuclear axis. Along the axis itself, there is a node, that is, a plane with no probability of finding an electron.

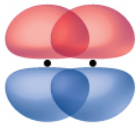
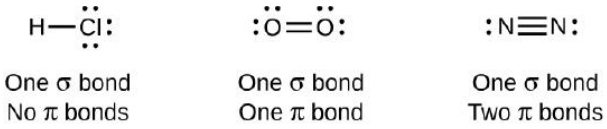


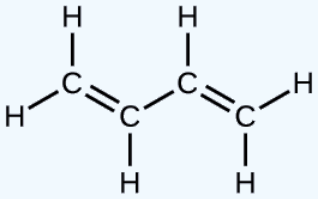
Figure **4.4.4**: Pi (π) bonds form from the side-by-side overlap of two *p* orbitals. The dots indicate the location of the nuclei.

While all single bonds are σ bonds, multiple bonds consist of both σ and π bonds. As the Lewis structures below suggest, O_2 contains a double bond, and N_2 contains a triple bond. The double bond consists of one σ bond and one π bond, and the triple bond consists of one σ bond and two π bonds. Between any two atoms, the first bond formed will always be a σ bond, but there can only be one σ bond in any one location. In any multiple bond, there will be one σ bond, and the remaining one or two bonds will be π bonds. These bonds are described in more detail later in this chapter.



As seen in Figure **4.4.1**, an average carbon-carbon single bond is 347 kJ/mol, while in a carbon-carbon double bond, the π bond increases the bond strength by 267 kJ/mol. Adding an additional π bond causes a further increase of 225 kJ/mol. We can see a similar pattern when we compare other σ and π bonds. Thus, each individual π bond is generally weaker than a corresponding σ bond between the same two atoms. In a σ bond, there is a greater degree of orbital overlap than in a π bond.

Example 4.4.1: Counting σ and π Bonds



Butadiene, C_4H_6, is used to make synthetic rubber. Identify the number of σ and π bonds contained in this molecule.

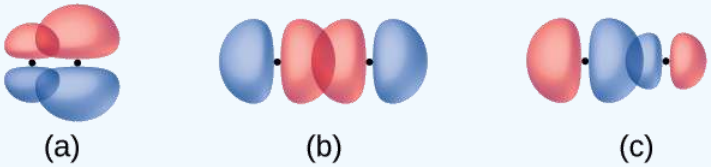
Solution

There are six σ C–H bonds and one σ C–C bond, for a total of seven from the single bonds. There are two double bonds that each have a π bond in addition to the σ bond. This gives a total nine σ and two π bonds overall.

Exercise 4.4.1

Identify each illustration as depicting a σ or π bond:

a. side-by-side overlap of a 4*p* and a 2*p* orbital
b. end-to-end overlap of a 4*p* and 4*p* orbital
c. end-to-end overlap of a 4*p* and a 2*p* orbital



Answer

(a) is a π bond with a node along the axis connecting the nuclei while (b) and (c) are σ bonds that overlap along the axis.

This page titled 4.4: Valence Bond Theory is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **8.1: Valence Bond Theory** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

4.5: Hybrid Atomic Orbitals

Learning Objectives

By the end of this section, you will be able to:

- Explain the concept of atomic orbital hybridization
- Determine the hybrid orbitals associated with various molecular geometries

Thinking in terms of overlapping atomic orbitals is one way for us to explain how chemical bonds form in diatomic molecules. However, to understand how molecules with more than two atoms form stable bonds, we require a more detailed model. As an example, let us consider the water molecule, in which we have one oxygen atom bonding to two hydrogen atoms. Oxygen has the electron configuration $1s^2 2s^2 2p^4$, with two unpaired electrons (one in each of the two 2*p* orbitals). Valence bond theory would predict that the two O–H bonds form from the overlap of these two 2*p* orbitals with the 1*s* orbitals of the hydrogen atoms. If this were the case, the bond angle would be 90°, as shown in Figure **4.5.1**, because *p* orbitals are perpendicular to each other. Experimental evidence shows that the bond angle is 104.5°, not 90°. The prediction of the valence bond theory model does not match the real-world observations of a water molecule; a different model is needed.

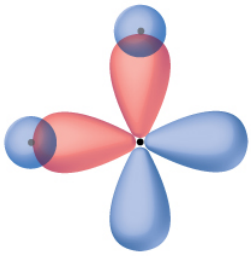


Figure **4.5.1**: The hypothetical overlap of two of the 2*p* orbitals on an oxygen atom (red) with the 1*s* orbitals of two hydrogen atoms (blue) would produce a bond angle of 90°. This is not consistent with experimental evidence.[1]

Quantum-mechanical calculations suggest why the observed bond angles in H_2O differ from those predicted by the overlap of the 1*s* orbital of the hydrogen atoms with the 2*p* orbitals of the oxygen atom. The mathematical expression known as the wave function, ψ, contains information about each orbital and the wavelike properties of electrons in an isolated atom. When atoms are bound together in a molecule, the wave functions combine to produce new mathematical descriptions that have different shapes. This process of combining the wave functions for atomic orbitals is called **hybridization** and is mathematically accomplished by the *linear combination of atomic orbitals*, LCAO, (a technique that we will encounter again later). The new orbitals that result are called **hybrid orbitals**. The valence orbitals in an *isolated* oxygen atom are a 2*s* orbital and three 2*p* orbitals. The valence orbitals in an oxygen atom in a water molecule differ; they consist of four equivalent hybrid orbitals that point approximately toward the corners of a tetrahedron (Figure **4.5.2**). Consequently, the overlap of the O and H orbitals should result in a tetrahedral bond angle (109.5°). The observed angle of 104.5° is experimental evidence for which quantum-mechanical calculations give a useful explanation: Valence bond theory must include a hybridization component to give accurate predictions.

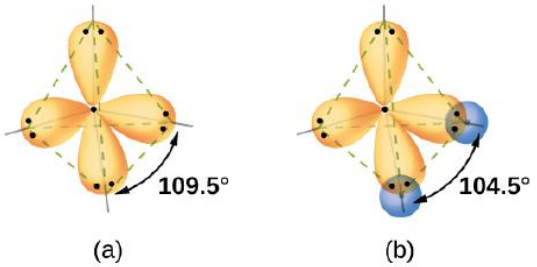


Figure **4.5.2**: (a) A water molecule has four regions of electron density, so VSEPR theory predicts a tetrahedral arrangement of hybrid orbitals. (b) Two of the hybrid orbitals on oxygen contain lone pairs, and the other two overlap with the 1*s* orbitals of hydrogen atoms to form the O–H bonds in H_2O. This description is more consistent with the experimental structure.

The following ideas are important in understanding hybridization:

1. Hybrid orbitals do not exist in isolated atoms. They are formed only in covalently bonded atoms

1. Hybrid orbitals do not exist in isolated atoms. They are formed only in covalently bonded atoms.
2. Hybrid orbitals have shapes and orientations that are very different from those of the atomic orbitals in isolated atoms.
3. A set of hybrid orbitals is generated by combining atomic orbitals. The number of hybrid orbitals in a set is equal to the number of atomic orbitals that were combined to produce the set.
4. All orbitals in a set of hybrid orbitals are equivalent in shape and energy.
5. The type of hybrid orbitals formed in a bonded atom depends on its electron-pair geometry as predicted by the VSEPR theory.
6. Hybrid orbitals overlap to form σ bonds. Unhybridized orbitals overlap to form π bonds.

In the following sections, we shall discuss the common types of hybrid orbitals.

4.5.1: *sp* Hybridization

The beryllium atom in a gaseous $BeCl_2$ molecule is an example of a central atom with no lone pairs of electrons in a linear arrangement of three atoms. There are two regions of valence electron density in the $BeCl_2$ molecule that correspond to the two covalent Be–Cl bonds. To accommodate these two electron domains, two of the Be atom's four valence orbitals will mix to yield two hybrid orbitals. This hybridization process involves mixing of the valence *s* orbital with one of the valence *p* orbitals to yield two equivalent ***sp* hybrid orbitals** that are oriented in a linear geometry (Figure **4.5.3**). In this figure, the set of *sp* orbitals appears similar in shape to the original *p* orbital, but there is an important difference. The number of atomic orbitals combined always equals the number of hybrid orbitals formed. The *p* orbital is one orbital that can hold up to two electrons. The *sp* set is two equivalent orbitals that point 180° from each other. The two electrons that were originally in the *s* orbital are now distributed to the two *sp* orbitals, which are half filled. In gaseous $BeCl_2$, these half-filled hybrid orbitals will overlap with orbitals from the chlorine atoms to form two identical σ bonds.

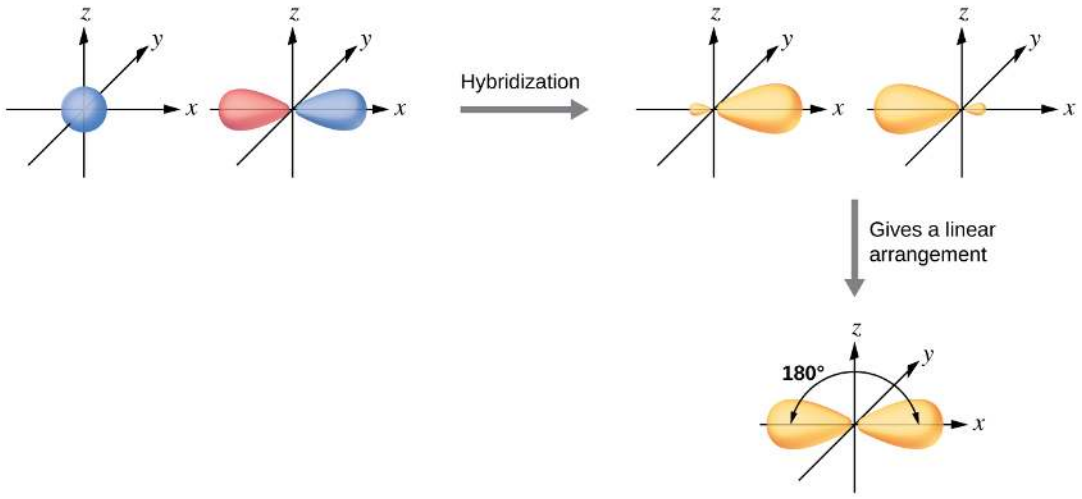


Figure **4.5.3**: Hybridization of an *s* orbital (blue) and a *p* orbital (red) of the same atom produces two *sp* hybrid orbitals (yellow). Each hybrid orbital is oriented primarily in just one direction. Note that each *sp* orbital contains one lobe that is significantly larger than the other. The set of two *sp* orbitals are oriented at 180°, which is consistent with the geometry for two domains.

We illustrate the electronic differences in an isolated Be atom and in the bonded Be atom in the orbital energy-level diagram in Figure **4.5.4**. These diagrams represent each orbital by a horizontal line (indicating its energy) and each electron by an arrow. Energy increases toward the top of the diagram. We use one upward arrow to indicate one electron in an orbital and two arrows (up and down) to indicate two electrons of opposite spin.

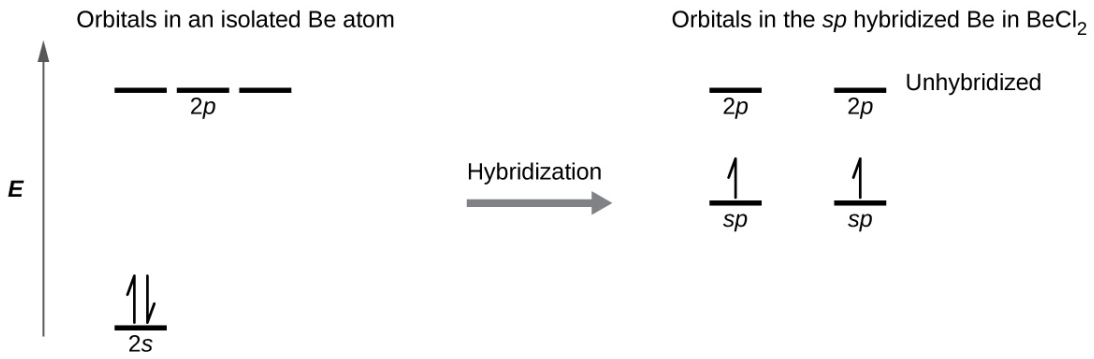


Figure **4.5.4**: This orbital energy-level diagram shows the *sp* hybridized orbitals on Be in the linear $BeCl_2$ molecule. Each of the two *sp* hybrid orbitals holds one electron and is thus half filled and available for bonding via overlap with a Cl 3*p* orbital.

When atomic orbitals hybridize, the valence electrons occupy the newly created orbitals. The Be atom had two valence electrons, so each of the *sp* orbitals gets one of these electrons. Each of these electrons pairs up with the unpaired electron on a chlorine atom when a hybrid orbital and a chlorine orbital overlap during the formation of the Be–Cl bonds.

Any central atom surrounded by just two regions of valence electron density in a molecule will exhibit *sp* hybridization. Other examples include the mercury atom in the linear $HgCl_2$ molecule, the zinc atom in $Zn(CH_3)_2$, which contains a linear C–Zn–C arrangement, and the carbon atoms in HCCH and CO_2.

Link to Learning

Check out the University of Wisconsin-Oshkosh website to learn about visualizing hybrid orbitals in three dimensions.

4.5.2: sp^2 Hybridization

The valence orbitals of a central atom surrounded by three regions of electron density consist of a set of three **sp^2 hybrid orbitals** and one unhybridized *p* orbital. This arrangement results from sp^2 hybridization, the mixing of one *s* orbital and two *p* orbitals to produce three identical hybrid orbitals oriented in a trigonal planar geometry (Figure **4.5.5**).

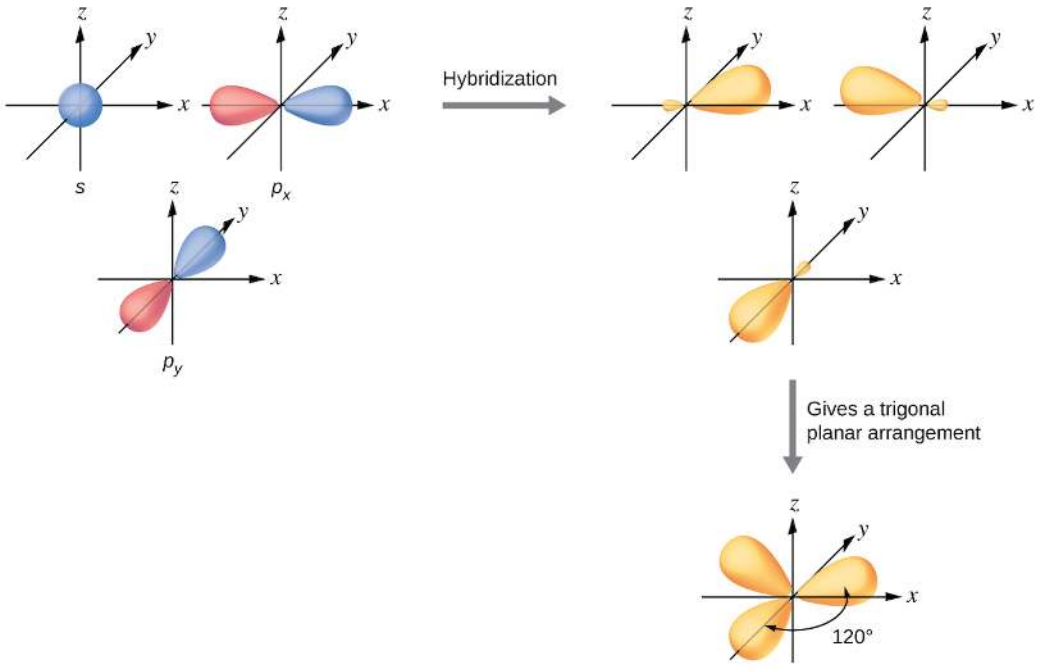


Figure **4.5.5**: The hybridization of an *s* orbital (blue) and two *p* orbitals (red) produces three equivalent sp^2 hybridized orbitals (yellow) oriented at 120° with respect to each other. The remaining unhybridized *p* orbital is not shown here, but is located along the z axis.

Although quantum mechanics yields the "plump" orbital lobes as depicted in Figure 4.5.5, sometimes for clarity these orbitals are drawn thinner and without the minor lobes, as in Figure 4.5.6, to avoid obscuring other features of a given illustration. We will use these "thinner" representations whenever the true view is too crowded to easily visualize.

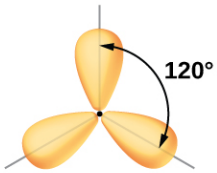


Figure 4.5.6: This alternate way of drawing the trigonal planar sp^2 hybrid orbitals is sometimes used in more crowded figures.

The observed structure of the borane molecule, BH_3, suggests sp^2 hybridization for boron in this compound. The molecule is trigonal planar, and the boron atom is involved in three bonds to hydrogen atoms (Figure 4.5.7). We can illustrate the comparison of orbitals and electron distribution in an isolated boron atom and in the bonded atom in BH_3 as shown in the orbital energy level diagram in Figure 4.5.8. We redistribute the three valence electrons of the boron atom in the three sp^2 hybrid orbitals, and each boron electron pairs with a hydrogen electron when B–H bonds form.

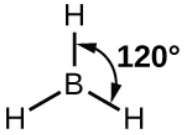


Figure 4.5.7: BH_3 is an electron-deficient molecule with a trigonal planar structure.

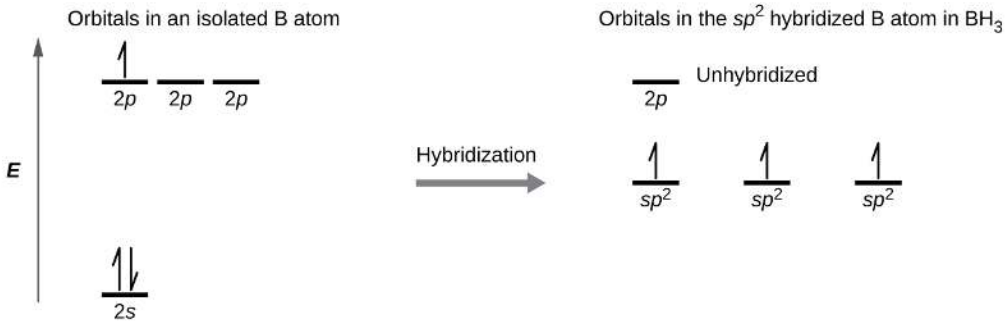


Figure 4.5.8: In an isolated B atom, there are one 2*s* and three 2*p* valence orbitals. When boron is in a molecule with three regions of electron density, three of the orbitals hybridize and create a set of three sp^2 orbitals and one unhybridized 2*p* orbital. The three half-filled hybrid orbitals each overlap with an orbital from a hydrogen atom to form three σ bonds in BH_3.

Any central atom surrounded by three regions of electron density will exhibit sp^2 hybridization. This includes molecules with a lone pair on the central atom, such as ClNO (Figure 4.5.9), or molecules with two single bonds and a double bond connected to the central atom, as in formaldehyde, CH_2O, and ethene, H_2CCH_2.

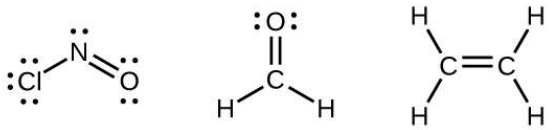


Figure 4.5.9: The central atom(s) in each of the structures shown contain three regions of electron density and are sp^2 hybridized. As we know from the discussion of VSEPR theory, a region of electron density contains all of the electrons that point in one direction. A lone pair, an unpaired electron, a single bond, or a multiple bond would each count as one region of electron density.

4.5.3: sp^3 Hybridization

The valence orbitals of an atom surrounded by a tetrahedral arrangement of bonding pairs and lone pairs consist of a set of four ***sp*^{3} hybrid orbitals**. The hybrids result from the mixing of one *s* orbital and all three *p* orbitals that produces four identical sp^3 hybrid orbitals (Figure 4.5.10). Each of these hybrid orbitals points toward a different corner of a tetrahedron.

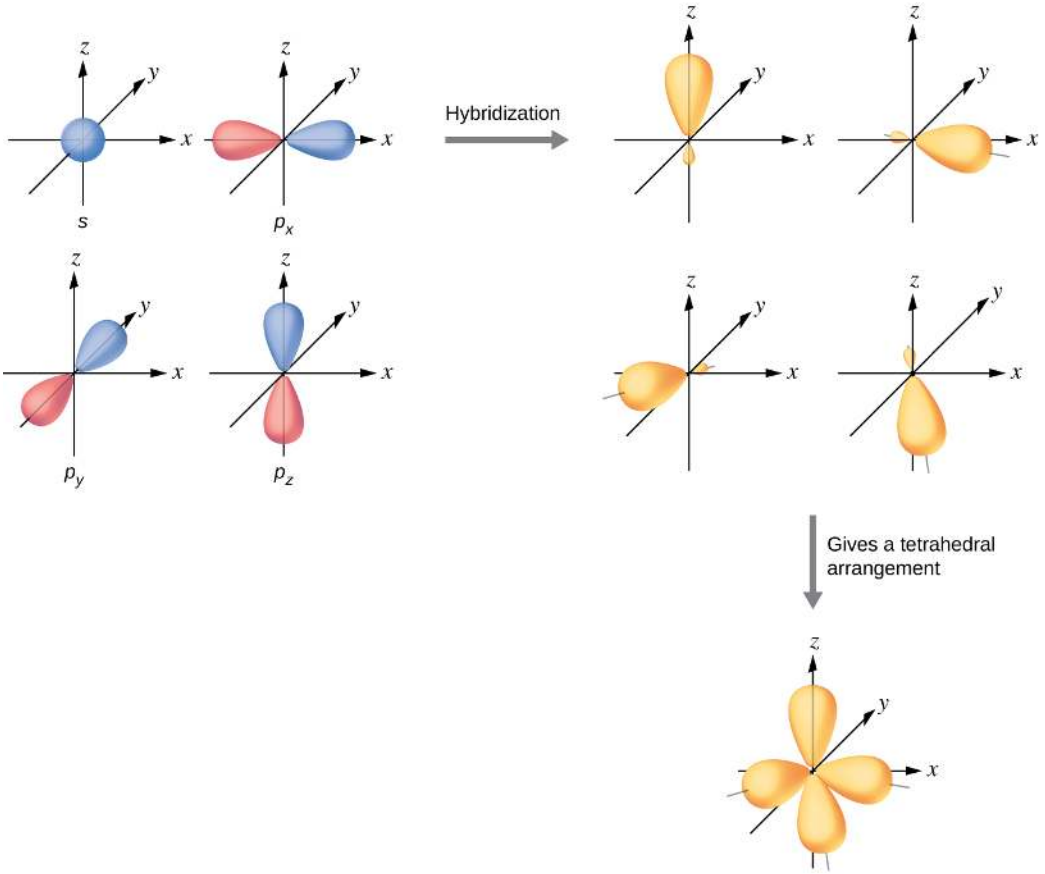


Figure 4.5.10: The hybridization of an *s* orbital (blue) and three *p* orbitals (red) produces four equivalent sp^3 hybridized orbitals (yellow) oriented at 109.5° with respect to each other.

A molecule of methane, CH_4, consists of a carbon atom surrounded by four hydrogen atoms at the corners of a tetrahedron. The carbon atom in methane exhibits sp^3 hybridization. We illustrate the orbitals and electron distribution in an isolated carbon atom and in the bonded atom in CH_4 in Figure 4.5.11. The four valence electrons of the carbon atom are distributed equally in the hybrid orbitals, and each carbon electron pairs with a hydrogen electron when the C–H bonds form.

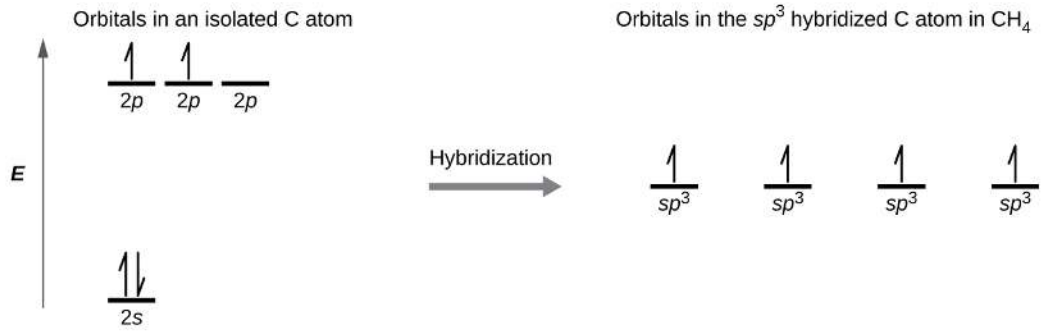


Figure 4.5.11: The four valence atomic orbitals from an isolated carbon atom all hybridize when the carbon bonds in a molecule like CH_4 with four regions of electron density. This creates four equivalent sp^3 hybridized orbitals. Overlap of each of the hybrid orbitals with a hydrogen orbital creates a C–H σ bond.

In a methane molecule, the 1*s* orbital of each of the four hydrogen atoms overlaps with one of the four sp^3 orbitals of the carbon atom to form a sigma (σ) bond. This results in the formation of four strong, equivalent covalent bonds between the carbon atom and each of the hydrogen atoms to produce the methane molecule, CH_4.

The structure of ethane, C_2H_6, is similar to that of methane in that each carbon in ethane has four neighboring atoms arranged at the corners of a tetrahedron—three hydrogen atoms and one carbon atom (Figure 4.5.12). However, in ethane an sp^3 orbital of one carbon atom overlaps end to end with an sp^3 orbital of a second carbon atom to form a σ bond between the two carbon atoms. Each

of the remaining sp^3 hybrid orbitals overlaps with an *s* orbital of a hydrogen atom to form carbon–hydrogen σ bonds. The structure and overall outline of the bonding orbitals of ethane are shown in Figure **4.5.12**. The orientation of the two CH_3 groups is not fixed relative to each other. Experimental evidence shows that rotation around σ bonds occurs easily.

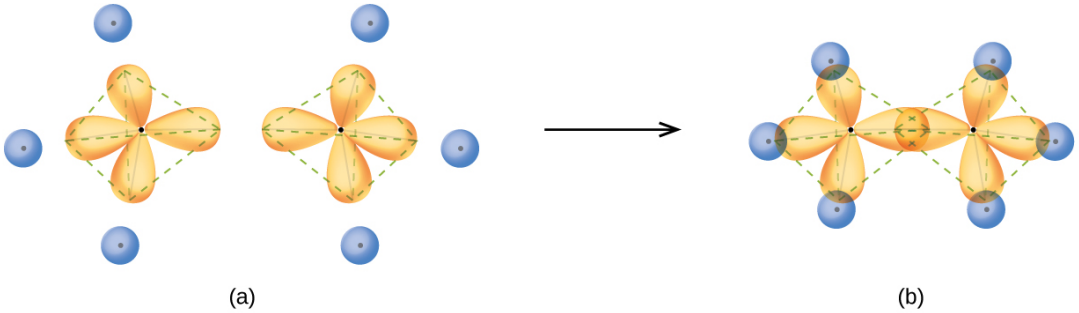


Figure **4.5.12**: (a) In the ethane molecule, C_2H_6, each carbon has four sp^3 orbitals. (b) These four orbitals overlap to form seven σ bonds.

An sp^3 hybrid orbital can also hold a lone pair of electrons. For example, the nitrogen atom in ammonia is surrounded by three bonding pairs and a lone pair of electrons directed to the four corners of a tetrahedron. The nitrogen atom is sp^3 hybridized with one hybrid orbital occupied by the lone pair.

The molecular structure of water is consistent with a tetrahedral arrangement of two lone pairs and two bonding pairs of electrons. Thus we say that the oxygen atom is sp^3 hybridized, with two of the hybrid orbitals occupied by lone pairs and two by bonding pairs. Since lone pairs occupy more space than bonding pairs, structures that contain lone pairs have bond angles slightly distorted from the ideal. Perfect tetrahedra have angles of 109.5°, but the observed angles in ammonia (107.3°) and water (104.5°) are slightly smaller. Other examples of sp^3 hybridization include CCl_4, PCl_3, and NCl_3.

4.5.4: sp^3d and sp^3d^2 Hybridization

To describe the five bonding orbitals in a trigonal bipyramidal arrangement, we must use five of the valence shell atomic orbitals (the *s* orbital, the three *p* orbitals, and one of the *d* orbitals), which gives five ***sp*^{3}*d* hybrid orbitals**. With an octahedral arrangement of six hybrid orbitals, we must use six valence shell atomic orbitals (the *s* orbital, the three *p* orbitals, and two of the *d* orbitals in its valence shell), which gives six ***sp*^{3}*d*^{2} hybrid orbitals**. These hybridizations are only possible for atoms that have *d* orbitals in their valence subshells (that is, not those in the first or second period).

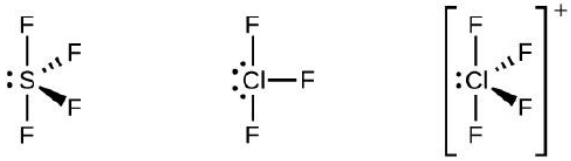


Figure **4.5.13**: The three compounds pictured exhibit sp^3d hybridization in the central atom and a trigonal bipyramid form. SF_4 and have one lone pair of electrons on the central atom, and ClF_3 has two lone pairs giving it the T-shape shown.

In a molecule of phosphorus pentachloride, PCl_5, there are five P–Cl bonds (thus five pairs of valence electrons around the phosphorus atom) directed toward the corners of a trigonal bipyramid. We use the 3*s* orbital, the three 3*p* orbitals, and one of the 3*d* orbitals to form the set of five sp^3d hybrid orbitals (Figure **4.5.14**) that are involved in the P–Cl bonds. Other atoms that exhibit sp^3d hybridization include the sulfur atom in SF_4 and the chlorine atoms in ClF_3 and in (The electrons on fluorine atoms are omitted for clarity.)

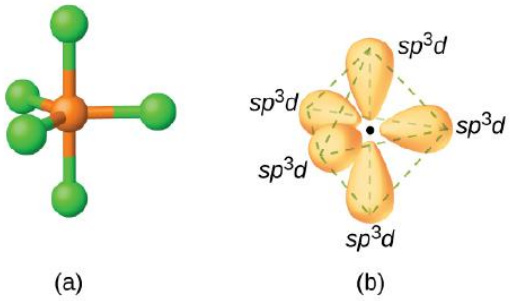


Figure **4.5.14**: (a) The five regions of electron density around phosphorus in PCl_5 require five hybrid sp^3d orbitals. (b) These orbitals combine to form a trigonal bipyramidal structure with each large lobe of the hybrid orbital pointing at a vertex. As before, there are also small lobes pointing in the opposite direction for each orbital (not shown for clarity).

The sulfur atom in sulfur hexafluoride, SF_6, exhibits sp^3d^2 hybridization. A molecule of sulfur hexafluoride has six bonding pairs of electrons connecting six fluorine atoms to a single sulfur atom. There are no lone pairs of electrons on the central atom. To bond six fluorine atoms, the 3*s* orbital, the three 3*p* orbitals, and two of the 3*d* orbitals form six equivalent sp^3d^2 hybrid orbitals, each directed toward a different corner of an octahedron. Other atoms that exhibit sp^3d^2 hybridization include the phosphorus atom in the iodine atom in the interhalogens IF_5, and the xenon atom in XeF_4.

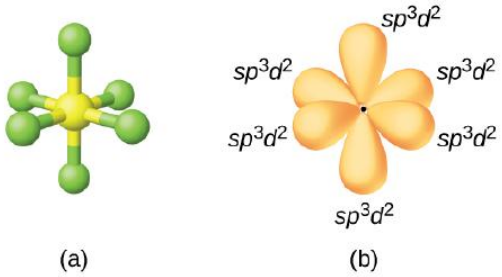


Figure **4.5.15**: (a) Sulfur hexafluoride, SF_6, has an octahedral structure that requires sp^3d^2 hybridization. (b) The six sp^3d^2 orbitals form an octahedral structure around sulfur. Again, the minor lobe of each orbital is not shown for clarity.

4.5.5: Assignment of Hybrid Orbitals to Central Atoms

The hybridization of an atom is determined based on the number of regions of electron density that surround it. The geometrical arrangements characteristic of the various sets of hybrid orbitals are shown in Figure **4.5.16**. These arrangements are identical to those of the electron-pair geometries predicted by VSEPR theory. VSEPR theory predicts the shapes of molecules, and hybrid orbital theory provides an explanation for how those shapes are formed. To find the hybridization of a central atom, we can use the following guidelines:

1. Determine the Lewis structure of the molecule.
2. Determine the number of regions of electron density around an atom using VSEPR theory, in which single bonds, multiple bonds, radicals, and lone pairs each count as one region.
3. Assign the set of hybridized orbitals from Figure **4.5.16** that corresponds to this geometry.

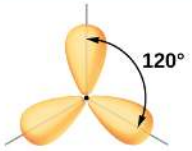
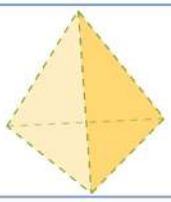
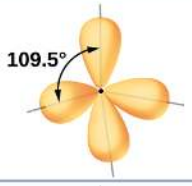
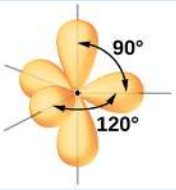
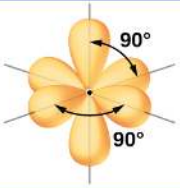
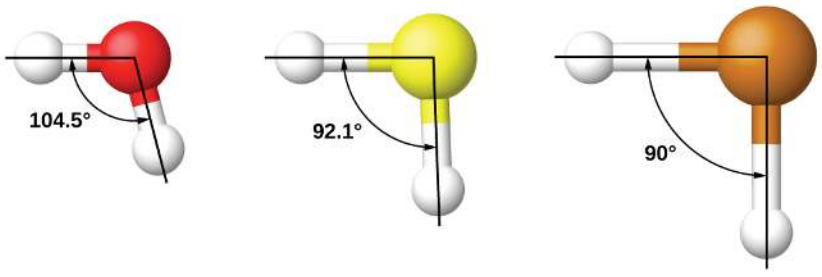
Regions of Electron Density	Arrangement		Hybridization	
2		linear	*sp*	
3		trigonal planar	sp^2	
4		tetrahedral	sp^3	
5		trigonal bipyramidal	sp^3d	
6		octahedral	sp^3d^2	

Figure 4.5.16: The shapes of hybridized orbital sets are consistent with the electron-pair geometries. For example, an atom surrounded by three regions of electron density is sp^2 hybridized, and the three sp^2 orbitals are arranged in a trigonal planar fashion.

It is important to remember that hybridization was devised to rationalize experimentally observed molecular geometries. The model works well for molecules containing small central atoms, in which the valence electron pairs are close together in space. However, for larger central atoms, the valence-shell electron pairs are farther from the nucleus, and there are fewer repulsions. Their compounds exhibit structures that are often not consistent with VSEPR theory, and hybridized orbitals are not necessary to explain the observed data. For example, we have discussed the H–O–H bond angle in H_2O, 104.5°, which is more consistent with sp^3 hybrid orbitals (109.5°) on the central atom than with 2*p* orbitals (90°). Sulfur is in the same group as oxygen, and H_2S has a similar Lewis structure. However, it has a much smaller bond angle (92.1°), which indicates much less hybridization on sulfur than oxygen. Continuing down the group, tellurium is even larger than sulfur, and for H_2Te, the observed bond angle (90°) is consistent with overlap of the 5*p* orbitals, without invoking hybridization. We invoke hybridization where it is necessary to explain the observed structures.

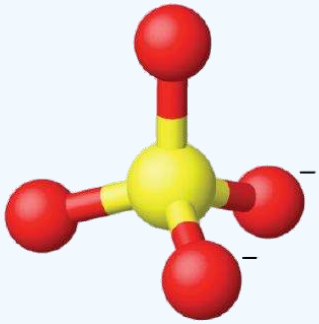


Example 4.5.1: Assigning Hybridization

Ammonium sulfate is important as a fertilizer. What is the hybridization of the sulfur atom in the sulfate ion,

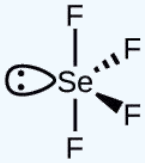
Solution

The Lewis structure of sulfate shows there are four regions of electron density. The hybridization is sp^3.



Exercise 4.5.1

What is the hybridization of the selenium atom in SeF_4?



Answer

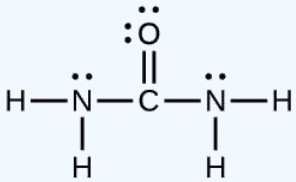
The selenium atom is sp^3d hybridized.

Example 4.5.2: Assigning Hybridization

Urea, $NH_2C(O)NH_2$, is sometimes used as a source of nitrogen in fertilizers. What is the hybridization of the carbon atom in urea?

Solution

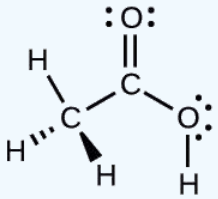
The Lewis structure of urea is



The carbon atom is surrounded by three regions of electron density, positioned in a trigonal planar arrangement. The hybridization in a trigonal planar electron pair geometry is sp^2 (Figure 4.5.16), which is the hybridization of the carbon atom in urea.

Exercise 4.5.1

Acetic acid, $H_3CC(O)OH$, is the molecule that gives vinegar its odor and sour taste. What is the hybridization of the two carbon atoms in acetic acid?



Answer

$H_3\underline{C}$, sp^3; $\underline{C}(O)OH$, sp^2

4.5.6: Footnotes

- 1Note that orbitals may sometimes be drawn in an elongated “balloon” shape rather than in a more realistic “plump” shape in order to make the geometry easier to visualize.

This page titled 4.5: Hybrid Atomic Orbitals is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **8.2: Hybrid Atomic Orbitals** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

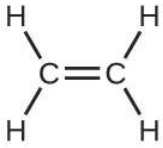
4.6: Multiple Bonds

Learning Objectives

By the end of this section, you will be able to:

- Describe multiple covalent bonding in terms of atomic orbital overlap
- Relate the concept of resonance to π-bonding and electron delocalization

The hybrid orbital model appears to account well for the geometry of molecules involving single covalent bonds. Is it also capable of describing molecules containing double and triple bonds? We have already discussed that multiple bonds consist of σ and π bonds. Next we can consider how we visualize these components and how they relate to hybrid orbitals. The Lewis structure of ethene, C_2H_4, shows us that each carbon atom is surrounded by one other carbon atom and two hydrogen atoms.



The three bonding regions form a trigonal planar electron-pair geometry. Thus we expect the σ bonds from each carbon atom are formed using a set of sp^2 hybrid orbitals that result from hybridization of two of the 2*p* orbitals and the 2*s* orbital (Figure **4.6.1**).

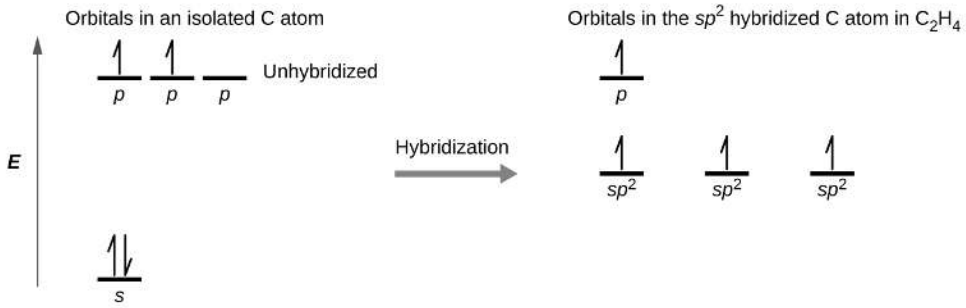


Figure **4.6.1**: In ethene, each carbon atom is sp^2 hybridized, and the sp^2 orbitals and the *p* orbital are singly occupied. The hybrid orbitals overlap to form σ bonds, while the *p* orbitals on each carbon atom overlap to form a π bond.

These orbitals form the C–H single bonds and the σ bond in the Figure **4.6.2**. The π bond in the C=C double bond results from the overlap of the third (remaining) 2p orbital on each carbon atom that is not involved in hybridization. This unhybridized p orbital (lobes shown in red and blue in Figure **4.6.2**) is perpendicular to the plane of the sp2 hybrid orbitals. Thus the unhybridized 2p orbitals overlap in a side-by-side fashion, above and below the internuclear axis (Figure **4.6.2**) and form a π bond.

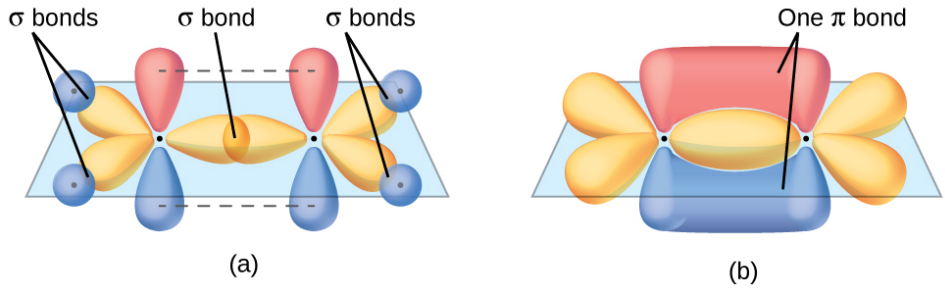


Figure **4.6.2**: In the ethene molecule, C_2H_4, there are (a) five σ bonds. One C–C σ bond results from overlap of sp^2 hybrid orbitals on the carbon atom with one sp^2 hybrid orbital on the other carbon atom. Four C–H bonds result from the overlap between the C atoms' sp^2 orbitals with *s* orbitals on the hydrogen atoms. (b) The π bond is formed by the side-by-side overlap of the two unhybridized *p* orbitals in the two carbon atoms. The two lobes of the π bond are above and below the plane of the σ system.

In an ethene molecule, the four hydrogen atoms and the two carbon atoms are all in the same plane. If the two planes of sp^2 hybrid orbitals tilted relative to each other, the *p* orbitals would not be oriented to overlap efficiently to create the π bond. The planar

configuration for the ethene molecule occurs because it is the most stable bonding arrangement. This is a significant difference between σ and π bonds; rotation around single (σ) bonds occurs easily because the end-to-end orbital overlap does not depend on the relative orientation of the orbitals on each atom in the bond. In other words, rotation around the internuclear axis does not change the extent to which the σ bonding orbitals overlap because the bonding electron density is symmetric about the axis. Rotation about the internuclear axis is much more difficult for multiple bonds; however, this would drastically alter the off-axis overlap of the π bonding orbitals, essentially breaking the π bond.

In molecules with *sp* hybrid orbitals, two unhybridized *p* orbitals remain on the atom (Figure **4.6.3**). We find this situation in acetylene, **H–C≡C–H** (Figure **4.6.4**), The remaining sp orbitals form σ bonds with hydrogen atoms. The two unhybridized *p* orbitals per carbon are positioned such that they overlap side by side and, hence, form two π bonds. The two carbon atoms of acetylene are thus bound together by one σ bond and two π bonds, giving a triple bond.

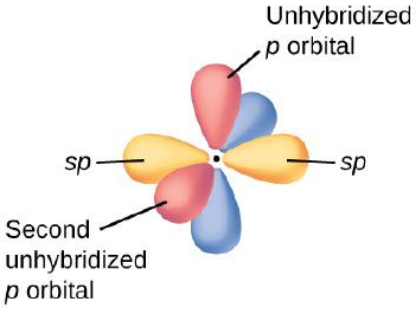


Figure **4.6.3**: Diagram of the two linear *sp* hybrid orbitals of a carbon atom, which lie in a straight line, and the two unhybridized *p* orbitals at perpendicular angles.

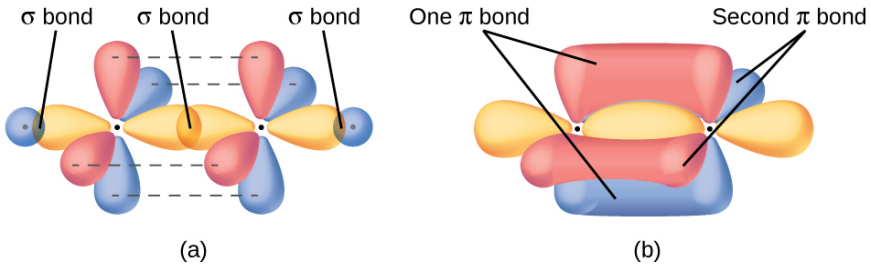


Figure **4.6.4**: (a) In the acetylene molecule, C_2H_2, there are two C–H σ bonds and a triple bond involving one C–C σ bond and two C–C π bonds. The dashed lines, each connecting two lobes, indicate the side-by-side overlap of the four unhybridized *p* orbitals. (b) This shows the overall outline of the bonds in C_2H_2. The two lobes of each of the π bonds are positioned across from each other around the line of the C–C σ bond.

Hybridization involves only σ bonds, lone pairs of electrons, and single unpaired electrons (radicals). Structures that account for these features describe the correct hybridization of the atoms. However, many structures also include resonance forms. Remember that resonance forms occur when various arrangements of π bonds are possible. Since the arrangement of π bonds involves only the unhybridized orbitals, resonance does not influence the assignment of hybridization.

For example, molecule benzene has two resonance forms (Figure **4.6.5**). We can use either of these forms to determine that each of the carbon atoms is bonded to three other atoms with no lone pairs, so the correct hybridization is sp^2. The electrons in the unhybridized *p* orbitals form π bonds. Neither resonance structure completely describes the electrons in the π bonds. They are not located in one position or the other, but in reality are delocalized throughout the ring. Valence bond theory does not easily address delocalization. Bonding in molecules with resonance forms is better described by molecular orbital theory. (See the next module.)

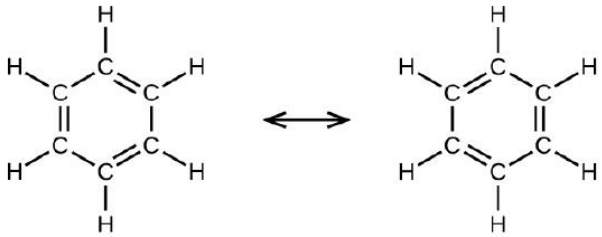


Figure **4.6.5**: Each carbon atom in benzene, C_6H_6, is sp^2 hybridized, independently of which resonance form is considered. The electrons in the π bonds are not located in one set of *p* orbitals or the other, but rather delocalized throughout the molecule.

Example 4.6.1: Assignment of Hybridization Involving Resonance

Some acid rain results from the reaction of sulfur dioxide with atmospheric water vapor, followed by the formation of sulfuric acid. Sulfur dioxide, SO_2, is a major component of volcanic gases as well as a product of the combustion of sulfur-containing coal. What is the hybridization of the S atom in SO_2?

Solution

The resonance structures of SO_2 are



The sulfur atom is surrounded by two bonds and one lone pair of electrons in either resonance structure. Therefore, the electron-pair geometry is trigonal planar, and the hybridization of the sulfur atom is sp^2.

Exercise 4.6.1

Another acid in acid rain is nitric acid, HNO_3, which is produced by the reaction of nitrogen dioxide, NO_2, with atmospheric water vapor. What is the hybridization of the nitrogen atom in NO_2? (Note: the lone electron on nitrogen occupies a hybridized orbital just as a lone pair would.)

Answer

sp^2

This page titled 4.6: Multiple Bonds is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **8.3: Multiple Bonds** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

4.7: Case Study- Chemical Bonding - Deciphering Drug Interactions through Lewis Structures

Introduction: Chemical bonds form the backbone of molecular interactions in all branches of chemistry, including the vital field of drug development. A key tool for understanding these interactions is the Lewis structure, a simple yet powerful diagrammatic representation of molecules. This case study explores the role of Lewis structures in predicting the behavior of pharmaceutical compounds.

Scenario: In the bustling corridors of Zenith Pharmaceuticals, Dr. Aisha Patel, a seasoned chemist, pores over the data sheets of an emerging drug compound. This new drug promises to revolutionize the treatment of hypertension, but before it can reach clinical trials, its molecular behavior must be thoroughly understood. Dr. Patel turns to the Lewis structure of the compound, seeking to unveil how its electrons are shared and arranged. Her goal is to predict how this molecule will interact with biological systems and to foresee any potential side effects that may not be immediately apparent from its basic composition.

The Importance of Lewis Structures: The Lewis structure serves as Dr. Patel's map, guiding her through the landscape of the drug's molecular architecture. It is more than dots and lines on paper—it represents the valence electrons forming chemical bonds and non-bonding pairs, which dictate the drug's reactivity and interaction with the body's biomolecules.

Case Study Questions:

1. **Explain the concept of a Lewis structure.**
2. **How can understanding chemical bonding aid in drug development?**

Hands-On Classroom Activities:

1. **Lewis Structure Puzzles:** In the activity "Lewis Structure Puzzles," students will solve puzzles that require the assembly of Lewis structures. This task aims to reinforce their comprehension of molecular geometry and the spatial arrangement of atoms within a molecule. It also reinforces their understanding of how molecules are pieced together and the significance of molecular shapes in chemistry.
2. **Drug Interaction Activity:** During the "Drug Interaction Activity," students are provided with various functional groups and are tasked with pairing them to investigate how the Lewis structures of these groups influence their interactions with biological targets. This exercise is designed to illuminate the relationship between the structural features of drug molecules and their potential binding affinities within biological systems.

Conclusion: As Dr. Patel annotates the Lewis structure with meticulous care, she is mindful of the impact her work will have on countless patients. The personal responsibility she feels drives her to ensure that every bond and electron is accounted for, knowing that even the smallest oversight could have significant repercussions. Her analysis of the Lewis structures is not just a routine task—it is a crucial step in the journey of a drug from the lab bench to the patient's bedside. The Lewis structure, a simple representation of atoms and electrons, becomes the foundation upon which safer and more effective therapeutic agents are built.

4.7: Case Study- Chemical Bonding - Deciphering Drug Interactions through Lewis Structures is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

4.8: 3D Printing Activity- VSEPR and Ionic/Metallic Solids Structures

Having physical models of shapes for students to examine while learning about VSEPR structures can be very valuable. Rather than make the models with molecular modeling kits, another option is to 3D print the models to pass around on the day(s) when VSEPR is being discussed. The models can be reused in future years once they are printed. The specific geometries of interest are those in Figure 4.3.6, including linear, trigonal planar, bent (<120), tetrahedral, trigonal pyramidal, bent (<109.5), trigonal bipyramidal, seesaw, t-shaped, linear, octahedral, square pyramidal, and square planar.

For those structures, .stl files exist and can be found on Thingverse. This user has all of the structures except for bent (<120): https://www.thingiverse.com/dclinch/designs. Another option is this full VSEPR kit: https://www.thingiverse.com/thing:4739079

4.8: 3D Printing Activity- VSEPR and Ionic/Metallic Solids Structures is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

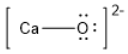
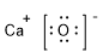
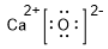
4.E: Exercises

Multiple Choice Questions

1. Which of the following is an ionic compound?

    a. PCl_5
    b. BaS
    c. NO_2
    d. XeF_4

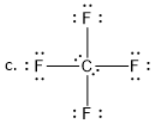
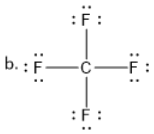
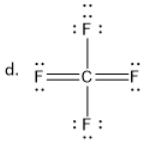
2. Which of the following shows the correct Lewis dot structure for CaO?

    a. 
    c. 
    b. 
    d. 

3. How many valence electrons are present in phosphate?

    a. 5
    b. 8
    c. 26
    d. 32

4. Which of the following shows the correct Lewis dot structure for CF_4?

    a. 
    c. 
    b. 
    d. 

5. What is the formal charge on bromide?

    a. −1
    b. 0
    c. 7
    d. 8

6. Which molecule requires octet expansion?

    a. CO_2
    b. NH_3
    c. CBr_4
    d. SF_6

7. Which central atom is sp^2 hybridized?

    a. BF_3
    b. CH_4
    c. NH_3
    d. H_2O

8. What is the hybridization of carbon in CH_2O?

    a. sp
    b. sp^2
    c. sp^3
    d. sp^4

9. Which molecule is polar?

a. CO_2
b. SO_2
c. CH_4
d. PCl_5

10. Which molecule is nonpolar?
    a. SF_6
    b. NH_3
    c. CS_2
    d. H_2O

Easy

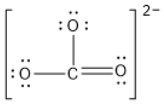
1. From their positions on the periodic table, order the atoms in terms of increasing electronegativity: F, Li, N
2. From their positions on the periodic table, order the atoms in terms of increasing electronegativity: Cl, Br, Rb
3. Predict which of the following compounds are ionic and which are covalent based on the location of their constituent atoms in the periodic table:
    a. MnO
    b. NCl_3
    c. $CoBr_2$
    d. K_2S
    e. CO
4. Predict which of the following compounds are ionic and which are covalent based on the location of their constituent atoms in the periodic table:
    a. CaF_2
    b. HI
    c. CaO
    d. IBr
    e. CO_2
5. Write the Lewis dot symbol for each of the following ions:
    a. As^{3-}
    b. I^-
    c. Be^{2+}
6. Write the Lewis dot symbol for each of the following ions:
    a. O^{2-}
    b. Ga^{3+}
    c. Li^+
7. Write the Lewis dot symbols of the ions in each of the following ionic compounds:
    a. MgS
    b. Al_2O_3
    c. $GaCl_3$
8. Write the Lewis dot symbols of the ions in each of the following ionic compounds:
    a. K_2O
    b. Li_3N
    c. KF
9. Write the Lewis dot structure for the following molecules:
    a. CCl_4
    b. CO_2
    c. O_2

10. Write the Lewis dot structure for the following molecules:
    a. N_2
    b. H_2O
    c. NH_3
11. What is the hybridization of the carbon atom in CH_4?
12. What is the hybridization of the carbon atom in CO_2?
13. Determine whether each of the following molecules is polar. Note: you should draw a Lewis dot structure of each molecule to determine your answer.
    a. CH_2Cl_2
    b. XeF_4
    c. PCl_3
14. Determine whether each of the following molecules is polar.
    a. SiF_4
    b. SCl_2
    c. HCN

Medium

1. Explain how a nonpolar covalent bond, a polar covalent bond, and an ionic bond differ from one another.
2. Which bond is more polar: N−O or N−F? Explain your reasoning.
3. Order the following bonds from least to most polar: Si-O, N-O, P-O.
4. Order the following bonds from least to most polar: C-Cl, C-Br, C-I.
5. Draw a Lewis dot structure for each of the following species.
    a. $COCl_2$
    b. PO_3^{3-}
    c. I^{3-}
6. Draw a Lewis dot structure for each of the following species.
    a. CN^-
    b. XeF_4
    c. NH_4^+
7. A Lewis dot structure for NO_2^- is shown below. What is the formal charge on N in this structure? What is the formal charge on each oxygen atom? What is the sum of the formal charges on all atoms in this structure?

8. A Lewis dot structure for CO_3^{2-} is shown below. What is the formal charge on C in this structure? What is the formal charge on each oxygen atom? What is the sum of the formal charges on all atoms in this structure?

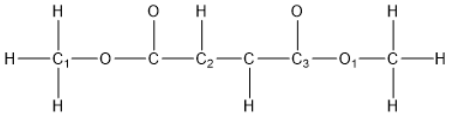


9. Draw a Lewis dot structure for each of the following molecules or ions. In all cases, you should draw the best Lewis dot structure allowing for octet expansion (when feasible) and following the rules of formal charges. Include resonance structures when relevant. Finally, state the VSEPR structure for each molecule or ion.
    a. $PClO_3$
    b. ClO_2-
    c. SO_3
10. Draw a Lewis dot structure for each of the following molecules or ions. In all cases, you should draw the best Lewis dot structure allowing for octet expansion (when feasible) and following the rules of formal charges. Include resonance structures when relevant. Finally, state the VSEPR structure for each molecule or ion.
    a. PO_4^{3-}

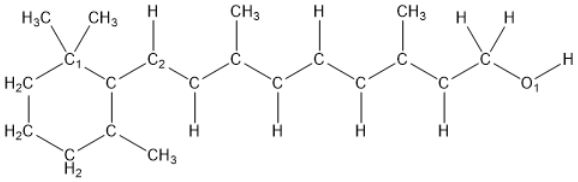
b. $SOCl_2$

c. ClO_3^-

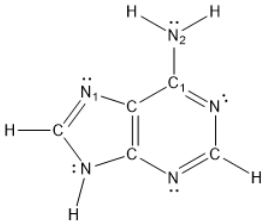
11. An incomplete Lewis dot structure of the molecule dimethyl fumarate, a medication used to treat multiple sclerosis, is shown below. Complete the Lewis dot structure by adding lone pairs and multiple bonds when needed. In addition, state the electron and local geometries around the atoms labeled C_1, C_2, C_3, and O_1.



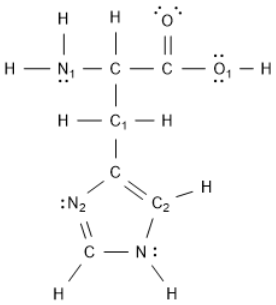
12. An incomplete Lewis dot structure of the molecule Vitamin A is shown below. Complete the Lewis dot structure by adding lone pairs and multiple bonds when needed. In addition, state the electron and local geometries around the atoms labeled C_1, C_2, and O_1. Note: In addition to the bonds shown, CH_2 indicates that the C atom is bonded to two H atoms and CH_3 indicates three bonds to H atoms.



13. The Lewis dot structure for the DNA base adenine is shown below. State the hybridization of N_1, N_2, and C_1. In addition, state the number of π (pi) bonds present in this molecule.



14. The Lewis dot structure for the amino acid histidine is shown below. State the hybridization of N_1, N_2, C_1, C_2, and O_1. In addition, state the number of π (pi) bonds present in this molecule.



15. Draw a Lewis dot structure for each of the following molecules, allowing for octet expansion (when feasible) and following the rules of formal charges. State the VSEPR structure for each molecule and state whether the molecule is polar or nonpolar.

a. $COCl_2$

b. IF_5

c. $RnCl_2$

16. Draw a Lewis dot structure for each of the following molecules, allowing for octet expansion (when feasible) and following the rules of formal charges. State the VSEPR structure for each molecule and state whether the molecule is polar or nonpolar.

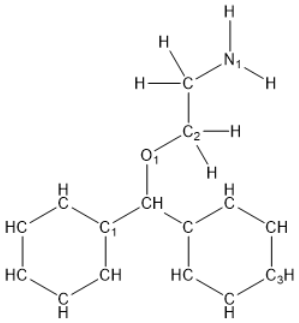
a. SO_2Cl_2

b. BF_3

c. ClF_3

Challenge

1. Draw all possible Lewis dot structures for an ion containing one atom each of O, C, and N, with an overall charge of -1. You should have a total of nine Lewis dot structures. Assign formal charges to all atoms in each structure. Based on your formal charge analysis, which structure is the best structure? Explain your choice.
2. An incomplete Lewis dot structure of the antihistamine diphenhydramine is shown below. Add lone pairs and multiple bonds as needed to complete this structure. In addition, state the electron and local geometries for the atoms labeled C_1, C_2, C_3, O_1, and N_1. In addition, state the hybridization for each of these numbered atoms.



Health-Related

1. Iodine (I_2) is a disinfectant. It is the active ingredient in topical disinfectants like Betadine. What is the Lewis structure of I_2? Is it polar?
2. Chlorine (Cl_2) is a disinfectant and bleaching agent that is used to treat water for drinking. What is the Lewis structure of Cl_2? Is it polar?
3. Dinitrogen monoxide, or nitrous oxide, is a linear molecule that has been used as an inhaled anesthetic. What is the Lewis structure of N_2O? Is it polar?
4. Chloroform, $CHCl_3$, is a small molecule with carbon as the central atom. It was used as an anesthetic in the 1800s but was abandoned due to toxicity and fatalities. What is the Lewis structure of chloroform? Is it polar?
5. Bicarbonate is an important ion in blood. What is the Lewis structure of bicarbonate? Show formal charges and include any resonance structures.
6. The nitrate anion is found in water and food and is present in our bodies in low amounts. What is the Lewis structure of nitrate? Show formal charges and include any resonance structures.

4.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

5: Unit Conversions

5.1: Density and Temperature

5.1.1: Mathematical Treatment of Measurement Results

5.2: Measurement Uncertainty, Accuracy, and Precision

5.3: Unit Conversions

5.4: Health Connections- Dosage Calculations

5.5: Case Study- Precision in Pediatric Care – The Imperative of Unit Conversion

5.E: Exercises

5: Unit Conversions is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

5.1: Density and Temperature

Learning Objectives

By the end of this section, you will be able to:

- Explain the process of measurement
- Identify the three basic parts of a quantity
- Describe the properties and units of length, mass, volume, density, temperature, and time
- Perform basic unit calculations and conversions in the metric and other unit systems

Measurements provide much of the information that informs the hypotheses, theories, and laws describing the behavior of matter and energy in both the macroscopic and microscopic domains of chemistry. Every measurement provides three kinds of information: the size or magnitude of the measurement (a number); a standard of comparison for the measurement (a unit); and an indication of the uncertainty of the measurement. While the number and unit are explicitly represented when a quantity is written, the uncertainty is an aspect of the measurement result that is more implicitly represented and will be discussed later.

The number in the measurement can be represented in different ways, including decimal form and scientific notation. (Scientific notation is also known as exponential notation; a review of this topic can be found in Appendix B.) For example, the maximum takeoff weight of a Boeing 777-200ER airliner is 298,000 kilograms, which can also be written as $2.98\ 10^5$ kg. The mass of the average mosquito is about 0.0000025 kilograms, which can be written as $2.5\ 10^{-6}$ kg.

Units, such as liters, pounds, and centimeters, are standards of comparison for measurements. A 2-liter bottle of a soft drink contains a volume of beverage that is twice that of the accepted volume of 1 liter. The meat used to prepare a 0.25-pound hamburger weighs one-fourth as much as the accepted weight of 1 pound. Without units, a number can be meaningless, confusing, or possibly life threatening. Suppose a doctor prescribes phenobarbital to control a patient's seizures and states a dosage of "100" without specifying units. Not only will this be confusing to the medical professional giving the dose, but the consequences can be dire: 100 mg given three times per day can be effective as an anticonvulsant, but a single dose of 100 g is more than 10 times the lethal amount.

The measurement units for seven fundamental properties ("base units") are listed in Table 5.1.1. The standards for these units are fixed by international agreement, and they are called the **International System of Units** or SI Units (from the French, *Le Système International d'Unités*). SI units have been used by the United States National Institute of Standards and Technology (NIST) since 1964. Units for other properties may be derived from these seven base units.

Table 5.1.1: Base Units of the SI System

Property Measured	Name of Unit	Symbol of Unit
length	meter	m
mass	kilogram	kg
time	second	s
temperature	kelvin	K
electric current	ampere	A
amount of substance	mole	mol
luminous intensity	candela	cd

Everyday measurement units are often defined as fractions or multiples of other units. Milk is commonly packaged in containers of 1 gallon (4 quarts), 1 quart (0.25 gallon), and one pint (0.5 quart). This same approach is used with SI units, but these fractions or multiples are always powers of 10. Fractional or multiple SI units are named using a prefix and the name of the base unit. For

example, a length of 1000 meters is also called a kilometer because the prefix *kilo* means “one thousand,” which in scientific notation is 10^3 (1 kilometer = 1000 m = 10^3 m). The prefixes used and the powers to which 10 are raised are listed in Table **5.1.2**.

Table **5.1.2**: Common Unit Prefixes

https://chem.libretexts.org/@go/page/449286

Prefix	Symbol	Factor	Example
femto	f	10^{-15}	1 femtosecond (fs) = 1 x 10^{-15} s (0.000000000000001 s)
pico	p	10^{-12}	1 picometer (pm) = 1 x 10^{-12} m (0.000000000001 m)
nano	n	10^{-9}	4 nanograms (ng) = 4 x 10^{-9} g (0.000000004 g)
micro	μ	10^{-6}	1 microliter (μL) = 1 x 10^{-6} L (0.000001 L)
milli	m	10^{-3}	2 millimoles (mmol) = 2 x 10^{-3} mol (0.002 mol)
centi	c	10^{-2}	7 centimeters (cm) = 7 x 10^{-2} m (0.07 m)
deci	d	10^{-1}	1 deciliter (dL) = 1 x 10^{-1} L (0.1 L)
kilo	k	10^{3}	1 kilometer (km) = 1 x 10^{3} m (1000 m)
mega	M	10^{6}	3 megahertz (MHz) = 3 x 10^{6} Hz (3,000,000 Hz)
g	G	10^{9}	8 gigayears (Gyr) = 8 x 10^{9} yr

Prefix	Symbol	Factor	Example
iga			(8,000,000,000 yr)
tera	T	10^{12}	5 terawatts (TW) = 5 x 10^{12} W (5,000,000,000,000 W)

Link to Learning

Need a refresher or more practice with scientific notation? Visit this site to go over the basics of scientific notation.

5.1.1: SI Base Units

The initial units of the metric system, which eventually evolved into the SI system, were established in France during the French Revolution. The original standards for the meter and the kilogram were adopted there in 1799 and eventually by other countries. This section introduces four of the SI base units commonly used in chemistry. Other SI units will be introduced in subsequent chapters.

5.1.1.1: Length

The standard unit of **length** in both the SI and original metric systems is the **meter** (m). A meter was originally specified as 1/10,000,000 of the distance from the North Pole to the equator. It is now defined as the distance light in a vacuum travels in 1/299,792,458 of a second. A meter is about 3 inches longer than a yard (Figure **5.1.1**); one meter is about 39.37 inches or 1.094 yards. Longer distances are often reported in kilometers (1 km = 1000 m = 10^3 m), whereas shorter distances can be reported in centimeters (1 cm = 0.01 m = 10^{-2} m) or millimeters (1 mm = 0.001 m = 10^{-3} m).

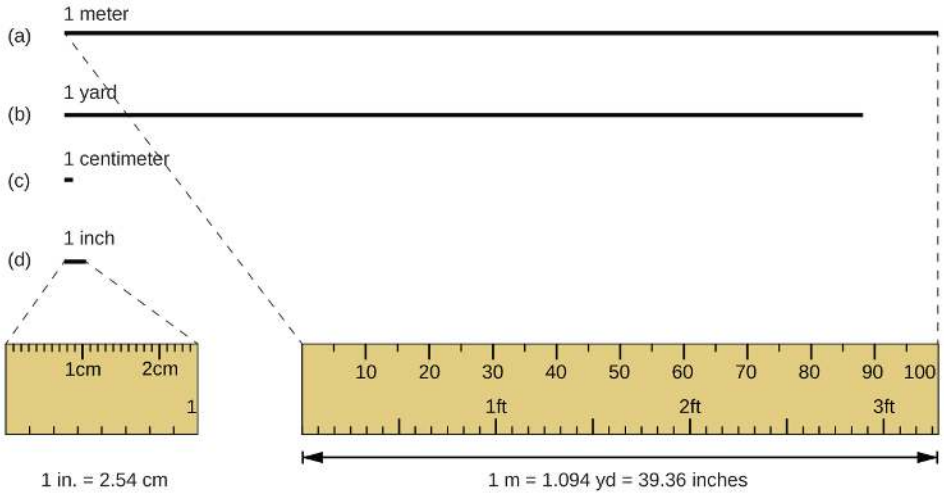


Figure **5.1.1**: The relative lengths of 1 m, 1 yd, 1 cm, and 1 in. are shown (not actual size), as well as comparisons of 2.54 cm and 1 in., and of 1 m and 1.094 yd.

5.1.1.2: Mass

The standard unit of mass in the SI system is the **kilogram** (kg). The kilogram was previously defined by the International Union of Pure and Applied Chemistry (IUPAC) as the mass of a specific reference object. This object was originally one liter of pure water, and more recently it was a metal cylinder made from a platinum-iridium alloy with a height and diameter of 39 mm (Figure **5.1.2**). In May 2019, this definition was changed to one that is based instead on precisely measured values of several fundamental physical constants.[1]. One kilogram is about 2.2 pounds. The gram (g) is exactly equal to 1/1000 of the mass of the kilogram (10^{-3} kg).



Figure **5.1.2**: This replica prototype kilogram as previously defined is housed at the National Institute of Standards and Technology (NIST) in Maryland. (credit: National Institutes of Standards and Technology)

5.1.1.3: Temperature

Temperature is an intensive property. The SI unit of temperature is the kelvin (K). The IUPAC convention is to use **kelvin** (all lowercase) for the word, K (uppercase) for the unit symbol, and neither the word “degree” nor the degree symbol (°). The degree **Celsius** (°C) is also allowed in the SI system, with both the word “degree” and the degree symbol used for Celsius measurements. Celsius degrees are the same magnitude as those of kelvin, but the two scales place their zeros in different places. Water freezes at 273.15 K (0 °C) and boils at 373.15 K (100 °C) by definition, and normal human body temperature is approximately 310 K (37 °C). The conversion between these two units and the Fahrenheit scale will be discussed later in this chapter.

5.1.1.4: Time

The SI base unit of time is the **second** (s). Small and large time intervals can be expressed with the appropriate prefixes; for example, 3 microseconds = 0.000003 s = 3 x 10^{-6} and 5 megaseconds = 5,000,000 s = 5 x 10^{6} s. Alternatively, hours, days, and years can be used.

5.1.2: Derived SI Units

We can derive many units from the seven SI base units. For example, we can use the base unit of length to define a unit of volume, and the base units of mass and length to define a unit of density.

5.1.2.1: Volume

Volume is the measure of the amount of space occupied by an object. The standard SI unit of volume is defined by the base unit of length (Figure **5.1.3**). The standard volume is a cubic meter (m^3), a cube with an edge length of exactly one meter. To dispense a cubic meter of water, we could build a cubic box with edge lengths of exactly one meter. This box would hold a cubic meter of water or any other substance.

A more commonly used unit of volume is derived from the decimeter (0.1 m, or 10 cm). A cube with edge lengths of exactly one decimeter contains a volume of one cubic decimeter (dm^3). A liter (L) is the more common name for the cubic decimeter. One **liter**

is about 1.06 quarts.

A **cubic centimeter** (cm^3) is the volume of a cube with an edge length of exactly one centimeter. The abbreviation **cc** (for **c**ubic **c**entimeter) is often used by health professionals. A cubic centimeter is equivalent to a milliliter (mL) and is 1/1000 of a liter.

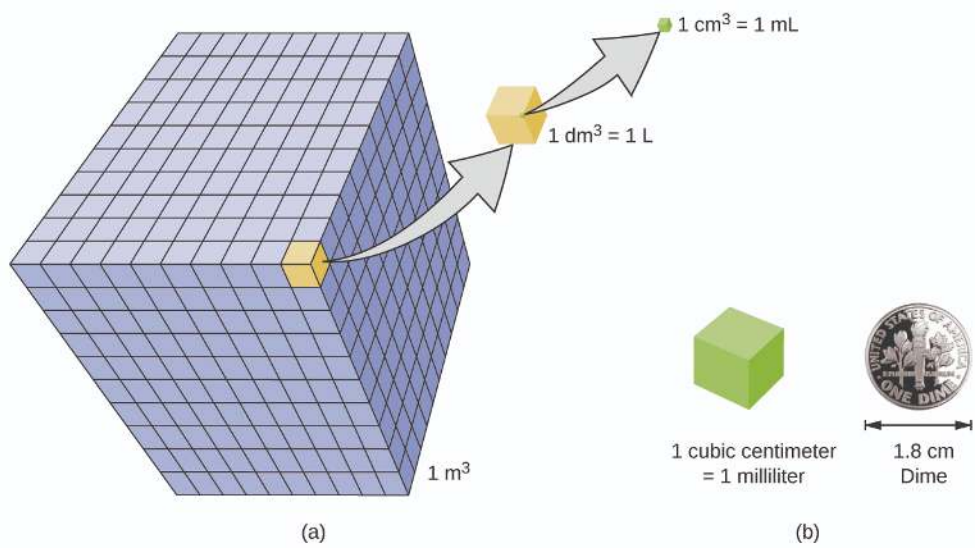


Figure **5.1.3**: (a) The relative volumes are shown for cubes of 1 m^3, 1 dm^3 (1 L), and 1 cm^3 (1 mL) (not to scale). (b) The diameter of a dime is compared relative to the edge length of a 1-cm^3 (1-mL) cube.

5.1.2.2: Density

We use the mass and volume of a substance to determine its density. Thus, the units of density are defined by the base units of mass and length.

The **density** of a substance is the ratio of the mass of a sample of the substance to its volume. The SI unit for density is the kilogram per cubic meter (kg/m^3). For many situations, however, this is an inconvenient unit, and we often use grams per cubic centimeter (g/cm^3) for the densities of solids and liquids, and grams per liter (g/L) for gases. Although there are exceptions, most liquids and solids have densities that range from about 0.7 g/cm^3 (the density of gasoline) to 19 g/cm^3 (the density of gold). The density of air is about 1.2 g/L. Table **5.1.3** shows the densities of some common substances.

Table **5.1.3**: Densities of Common Substances

Solids	Liquids	Gases (at 25 °C and 1 atm)
ice (at 0 °C) 0.92 g/cm^3	water 1.0 g/cm^3	dry air 1.20 g/L
oak (wood) 0.60–0.90 g/cm^3	ethanol 0.79 g/cm^3	oxygen 1.31 g/L
iron 7.9 g/cm^3	acetone 0.79 g/cm^3	nitrogen 1.14 g/L
copper 9.0 g/cm^3	glycerin 1.26 g/cm^3	carbon dioxide 1.80 g/L
lead 11.3 g/cm^3	olive oil 0.92 g/cm^3	helium 0.16 g/L
silver 10.5 g/cm^3	gasoline 0.70–0.77 g/cm^3	neon 0.83 g/L
gold 19.3 g/cm^3	mercury 13.6 g/cm^3	radon 9.1 g/L

While there are many ways to determine the density of an object, perhaps the most straightforward method involves separately finding the mass and volume of the object, and then dividing the mass of the sample by its volume. In the following example, the mass is found directly by weighing, but the volume is found indirectly through length measurements.

$$\text{density} = \frac{\text{mass}}{\text{volume}} \tag{5.1.1}$$

Example 5.1.1: Calculation of Density

Gold—in bricks, bars, and coins—has been a form of currency for centuries. In order to swindle people into paying for a brick of gold without actually investing in a brick of gold, people have considered filling the centers of hollow gold bricks with lead to fool buyers into thinking that the entire brick is gold. It does not work: Lead is a dense substance, but its density is not as great as that of gold, 19.3 g/cm^3. What is the density of lead if a cube of lead has an edge length of 2.00 cm and a mass of 90.7 g?

Solution

The density of a substance can be calculated by dividing its mass by its volume. The volume of a cube is calculated by cubing the edge length.

$$\text{volume of lead cube } = 2.00\ \text{cm} \times 2.00\ \text{cm} \times 2.00\ \text{cm} = 8.00\ \text{cm}^3$$

$$\text{density } = \frac{\text{mass}}{\text{volume}} = \frac{90.7\ \text{g}}{8.00\ \text{cm}^3} = 11.3\ \text{g/cm}^3$$

(We will discuss the reason for rounding to the first decimal place in the next section.)

Exercise 5.1.1

a. To three decimal places, what is the volume of a cube (cm^3) with an edge length of 0.843 cm?
b. If the cube in part (a) is copper and has a mass of 5.34 g, what is the density of copper to two decimal places?

Answer

a. 0.599 cm^3
b. 8.91 g/cm^3

Link to Learning

To learn more about the relationship between mass, volume, and density, use this interactive simulator to explore the density of different materials.

Example 5.1.2: Using Displacement of Water to Determine Density

This exercise uses a simulation to illustrate an alternative approach to the determination of density that involves measuring the object's volume via displacement of water. Use the simulator to determine the densities iron and wood.

Solution

Click the "turn fluid into water" button in the simulator to adjust the density of liquid in the beaker to 1.00 g/mL. Remove the red block from the beaker and note the volume of water is 25.5 mL. Select the iron sample by clicking "iron" in the table of materials at the bottom of the screen, place the iron block on the balance pan, and observe its mass is 31.48 g. Transfer the iron block to the beaker and notice that it sinks, displacing a volume of water equal to its own volume and causing the water level to rise to 29.5 mL. The volume of the iron block is therefore:

$$v_{\text{iron}} = 29.5mL - 25.5mL = 4.0mL$$

The density of the iron is then calculated to be:

$$\text{density } = \frac{\text{mass}}{\text{volume}} = \frac{31.48\ \text{g}}{4.0\ \text{mL}} = 7.9\ \text{g/mL}$$

Remove the iron block from the beaker, change the block material to wood, and then repeat the mass and volume measurements. Unlike iron, the wood block does not sink in the water but instead floats on the water's surface. To measure its volume, drag it beneath the water's surface so that it is fully submerged.

$$\text{density} = \frac{\text{mass}}{\text{volume}} = \frac{1.95\,\text{g}}{3.0\,\text{mL}} = 0.65\,\text{g/mL}$$

Note: The sink versus float behavior illustrated in this example demonstrates the property of “buoyancy”.

? Exercise 5.1.2

Following the water displacement approach, use the simulator to measure the density of the foam sample.

Answer

0.230 g/mL

5.1.3: Footnotes

- 1For details see https://www.nist.gov/pml/weights-and.../si-units-mass

---

This page titled 5.1: Density and Temperature is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.4: Measurements** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

5.1.1: Mathematical Treatment of Measurement Results

Learning Objectives

By the end of this section, you will be able to:

- Explain the dimensional analysis (factor label) approach to mathematical calculations involving quantities
- Use dimensional analysis to carry out unit conversions for a given property and computations involving two or more properties

It is often the case that a quantity of interest may not be easy (or even possible) to measure directly but instead must be calculated from other directly measured properties and appropriate mathematical relationships. For example, consider measuring the average speed of an athlete running sprints. This is typically accomplished by measuring the *time* required for the athlete to run from the starting line to the finish line, and the *distance* between these two lines, and then computing *speed* from the equation that relates these three properties:

$$\text{speed} = \frac{\text{distance}}{\text{time}}$$

An Olympic-quality sprinter can run 100 m in approximately 10 s, corresponding to an average speed of

$$\frac{100\,\text{m}}{10\,\text{s}} = 10\,\text{m/s}$$

(For this and the next calculation, assume the trailing zeros are significant digits.) Note that this simple arithmetic involves dividing the numbers of each measured quantity to yield the number of the computed quantity (100/10 = 10) *and likewise* dividing the units of each measured quantity to yield the unit of the computed quantity (m/s = m/s). Now, consider using this same relation to predict the time required for a person running at this speed to travel a distance of 25 m. The same relation among the three properties is used, but in this case, the two quantities provided are a speed (10 m/s) and a distance (25 m). To yield the sought property, time, the equation must be rearranged appropriately:

$$\text{time} = \frac{\text{distance}}{\text{speed}}$$

The time can then be computed as:

$$\frac{25\,\text{m}}{10\,\text{m/s}} = 2.5\,\text{s}$$

Again, arithmetic on the numbers (25/10 = 2.5) was accompanied by the same arithmetic on the units (m/(m/s) = s) to yield the number and unit of the result, 2.5 s. Note that, just as for numbers, when a unit is divided by an identical unit (in this case, m/m), the result is "1"—or, as commonly phrased, the units "cancel."

These calculations are examples of a versatile mathematical approach known as **dimensional analysis** (or the **factor-label method**). Dimensional analysis is based on this premise: *the units of quantities must be subjected to the same mathematical operations as their associated numbers*. This method can be applied to computations ranging from simple unit conversions to more complex, multi-step calculations involving several different quantities.

5.1.1.1: Conversion Factors and Dimensional Analysis

A ratio of two equivalent quantities expressed with different measurement units can be used as a **unit conversion factor**. For example, the lengths of 2.54 cm and 1 in. are equivalent (by definition), and so a unit conversion factor may be derived from the ratio,

$$\frac{2.54\,\text{cm}}{1\,\text{in.}}\,(2.54\,\text{cm} = 1\,\text{in.}) \text{ or } 2.54\frac{\text{cm}}{\text{in.}}$$

Several other commonly used conversion factors are given in Example **5.1.1.1**.

Example **5.1.1.1**: Common Conversion Factors

Length	Volume	Mass
1 m = 1.0936 yd	1 L = 1.0567 qt	1 kg = 2.2046 lb
1 in. = 2.54 cm (exact)	1 qt = 0.94635 L	1 lb = 453.59 g
1 km = 0.62137 mi	1 ft^3 = 28.317 L	1 (avoirdupois) oz = 28.349 g
1 mi = 1609.3 m	1 tbsp = 14.787 mL	1 (troy) oz = 31.103 g

When a quantity (such as distance in inches) is multiplied by an appropriate unit conversion factor, the quantity is converted to an equivalent value with different units (such as distance in centimeters). For example, a basketball player's vertical jump of 34 inches can be converted to centimeters by:

$$34 \cancel{\text{in.}} \times \frac{2.54\,\text{cm}}{1\,\cancel{\text{in.}}} = 86\,\text{cm}$$

Since this simple arithmetic involves *quantities*, the premise of dimensional analysis requires that we multiply both *numbers and units*. The numbers of these two quantities are multiplied to yield the number of the product quantity, 86, whereas the units are multiplied to yield . Just as for numbers, a ratio of identical units is also numerically equal to one, and the unit product thus simplifies to *cm*. (When identical units divide to yield a factor of 1, they are said to "cancel.") Dimensional analysis may be used to confirm the proper application of unit conversion factors as demonstrated in the following example.

✔ Example 5.1.1.1: Using a Unit Conversion Factor

The mass of a competition frisbee is 125 g. Convert its mass to ounces using the unit conversion factor derived from the relationship 1 oz = 28.349 g (Example **5.1.1.1**).

Solution

Given the conversion factor, the mass in ounces may be derived using an equation similar to the one used for converting length from inches to centimeters.

$$x\,oz = 125g \times \text{ unit conversion factor}$$

The unit conversion factor may be represented as:

$$\frac{1\,\text{oz}}{28.349\,\text{g}} \text{ and } \frac{28.349\,\text{g}}{1\,\text{oz}}$$

The correct unit conversion factor is the ratio that cancels the units of grams and leaves ounces.

$$\begin{aligned} x\,\text{oz} &= 125\,\text{g} \times \frac{1\,\text{oz}}{28.349\,\text{g}} \\ &= \left(\frac{125}{28.349}\right)\,\text{oz} \\ &= 4.41\,\text{oz (three significant figures)} \end{aligned}$$

? Exercise 5.1.1.1

Convert a volume of 9.345 qt to liters.

Answer

8.844 L

Beyond simple unit conversions, the factor-label method can be used to solve more complex problems involving computations. Regardless of the details, the basic approach is the same—all the *factors* involved in the calculation must be appropriately oriented

to ensure that their *labels* (units) will appropriately cancel and/or combine to yield the desired unit in the result. As your study of chemistry continues, you will encounter many opportunities to apply this approach.

Example 5.1.1.2: Computing Quantities from Measurement Results and Known Mathematical Relations

What is the density of common antifreeze in units of g/mL? A 4.00-qt sample of the antifreeze weighs 9.26 lb.

Solution

Since $\text{density} = \frac{\text{mass}}{\text{volume}}$, we need to divide the mass in grams by the volume in milliliters. In general: the number of units of B = the number of units of A × unit conversion factor. The necessary conversion factors are given in Example 5.1.1.1: 1 lb = 453.59 g; 1 L = 1.0567 qt; 1 L = 1,000 mL. Mass may be converted from pounds to grams as follows:

$$9.26 \cancel{\text{lb}} \times \left(\frac{453.59\,\text{g}}{1\,\cancel{\text{lb}}} \right) = 4.20 \times 10^3\,\text{g}$$

Volume may be converted from quarts to milliliters via two steps:

Step 1: Convert quarts to liters.

$$4.00\,\cancel{\text{qt}} \times \left(\frac{1\,\text{L}}{1.0567\,\cancel{\text{qt}}} \right) = 3.78\,\text{L}$$

Step 2: Convert liters to milliliters.

$$3.78\,\cancel{\text{L}} \times \left(\frac{1000\,\text{mL}}{1\,\cancel{\text{L}}} \right) = 3.78 \times 10^3\,\text{mL}$$

Then,

$$\text{density} = \frac{4.20 \times 10^3\,\text{g}}{3.78 \times 10^3\,\text{mL}} = 1.11\,\text{g/mL}$$

Alternatively, the calculation could be set up in a way that uses three unit conversion factors sequentially as follows:

$$\frac{9.26\,\cancel{\text{lb}}}{4.00\,\cancel{\text{qt}}} \times \frac{453.59\,\text{g}}{1\,\cancel{\text{lb}}} \times \frac{1.0567\,\cancel{\text{qt}}}{1\,\cancel{\text{L}}} \times \frac{1\,\cancel{\text{L}}}{1000\,\text{mL}} = 1.11\,\text{g/mL}$$

Exercise 5.1.1.2

What is the volume in liters of 1.000 oz, given that 1 L = 1.0567 qt and 1 qt = 32 oz (exactly)?

Answer

2.956×10^{-2} L

Example 5.1.1.3: Computing Quantities from Measurement Results and Known Mathematical Relations

While being driven from Philadelphia to Atlanta, a distance of about 1250 km, a 2014 Lamborghini Aventador Roadster uses 213 L gasoline.

a. What (average) fuel economy, in miles per gallon, did the Roadster get during this trip?
b. If gasoline costs $3.80 per gallon, what was the fuel cost for this trip?

Solution

(a) First convert distance from kilometers to miles:

$$1250 \cancel{\text{km}} \times \frac{0.62137\,\text{mi}}{1\,\cancel{\text{km}}} = 777\,\text{mi}$$

and then convert volume from liters to gallons:

$$213\,\cancel{\text{L}} \times \frac{1.0567\,\cancel{\text{qt}}}{1\,\cancel{\text{L}}} \times \frac{1\,\text{gal}}{4\,\cancel{\text{qt}}} = 56.3\,\text{gal}$$

Finally,

$$\text{(average) mileage} = \frac{777\,\text{mi}}{56.3\,\text{gal}} = 13.8\ \text{miles / gallon} = 13.8, \text{mpg}$$

Alternatively, the calculation could be set up in a way that uses all the conversion factors sequentially, as follows:

$$\frac{1250\,\cancel{\text{km}}}{213\,\cancel{\text{L}}} \times \frac{0.62137\,\text{mi}}{1\,\cancel{\text{km}}} \times \frac{1\,\cancel{\text{L}}}{1.0567\,\cancel{\text{qt}}} \times \frac{4\,\cancel{\text{qt}}}{1\,\text{gal}} = 13.8\,\text{mpg}$$

(b) Using the previously calculated volume in gallons, we find:

$$56.3\,\cancel{\text{gal}} \times \frac{\$3.80}{1\,\cancel{\text{gal}}} = \$214$$

? Exercise 5.1.1.3

A Toyota Prius Hybrid uses 59.7 L gasoline to drive from San Francisco to Seattle, a distance of 1300 km (two significant digits).

a. What (average) fuel economy, in miles per gallon, did the Prius get during this trip?
b. If gasoline costs $3.90 per gallon, what was the fuel cost for this trip?

Answer

a. 51 mpg
b. $62

5.1.1.2: Conversion of Temperature Units

We use the word **temperature** to refer to the hotness or coldness of a substance. One way we measure a change in temperature is to use the fact that most substances expand when their temperature increases and contract when their temperature decreases. The liquid in a common glass thermometer changes its volume as the temperature changes, and the position of the trapped liquid's surface along a printed scale may be used as a measure of temperature.

Temperature scales are defined relative to selected reference temperatures: Two of the most commonly used are the freezing and boiling temperatures of water at a specified atmospheric pressure. On the Celsius scale, 0 °C is defined as the freezing temperature of water and 100 °C as the boiling temperature of water. The space between the two temperatures is divided into 100 equal intervals, which we call degrees. On the **Fahrenheit** scale, the freezing point of water is defined as 32 °F and the boiling temperature as 212 °F. The space between these two points on a Fahrenheit thermometer is divided into 180 equal parts (degrees).

Defining the Celsius and Fahrenheit temperature scales as described in the previous paragraph results in a slightly more complex relationship between temperature values on these two scales than for different units of measure for other properties. Most measurement units for a given property are directly proportional to one another (y = mx). Using familiar length units as one example:

$$\text{length in feet} = \left(\frac{1ft}{12in.}\right) \times \text{length in inches}$$

where y = length in feet, x = length in inches, and the proportionality constant, m, is the conversion factor. The Celsius and Fahrenheit temperature scales, however, do not share a common zero point, and so the relationship between these two scales is a

linear one rather than a proportional one (y = mx + b). Consequently, converting a temperature from one of these scales into the other requires more than simple multiplication by a conversion factor, m; it also must take into account differences in the scales' zero points (b).

The linear equation relating Celsius and Fahrenheit temperatures is easily derived from the two temperatures used to define each scale. Representing the Celsius temperature as *x* and the Fahrenheit temperature as *y*, the slope, *m*, is computed to be:

$$m = \frac{\Delta y}{\Delta x} = \frac{212^\circ F - 32^\circ F}{100^\circ C - 0^\circ C} = \frac{180^\circ F}{100^\circ C} = \frac{9^\circ F}{5^\circ C}$$

The *y*-intercept of the equation, *b*, is then calculated using either of the equivalent temperature pairs, (100 °C, 212 °F) or (0 °C, 32 °F), as:

$$b = y - mx = 32^\circ F - \frac{9^\circ F}{5^\circ C} \times 0^\circ C = 32^\circ F$$

The equation relating the temperature (T) scales is then:

$$T^\circ F = \left(\frac{9^\circ F}{5^\circ C} \times T^\circ C\right) + 32^\circ F$$

An abbreviated form of this equation that omits the measurement units is:

$$T^\circ F = \left(\frac{9}{5} \times T^\circ C\right) + 32$$

Rearrangement of this equation yields the form useful for converting from Fahrenheit to Celsius:

$$T^\circ F = \left(\frac{9}{5} \times T^\circ C\right) + 32$$

As mentioned earlier in this chapter, the SI unit of temperature is the kelvin (K). Unlike the Celsius and Fahrenheit scales, the kelvin scale is an absolute temperature scale in which 0 (zero) K corresponds to the lowest temperature that can theoretically be achieved. Since the kelvin temperature scale is absolute, a degree symbol is not included in the unit abbreviation, K. The early 19th-century discovery of the relationship between a gas's volume and temperature suggested that the volume of a gas would be zero at −273.15 °C. In 1848, British physicist William Thompson, who later adopted the title of Lord Kelvin, proposed an absolute temperature scale based on this concept (further treatment of this topic is provided in this text's chapter on gases).

The freezing temperature of water on this scale is 273.15 K and its boiling temperature is 373.15 K. Notice the numerical difference in these two reference temperatures is 100, the same as for the Celsius scale, and so the linear relation between these two temperature scales will exhibit a slope of . Following the same approach, the equations for converting between the kelvin and Celsius temperature scales are derived to be:

$$T_K = T^\circ C + 273.15$$
$$T^{\circ C} = T_K - 273.15$$

The 273.15 in these equations has been determined experimentally, so it is not exact. Figure 5.1.1.1: shows the relationship among the three temperature scales.

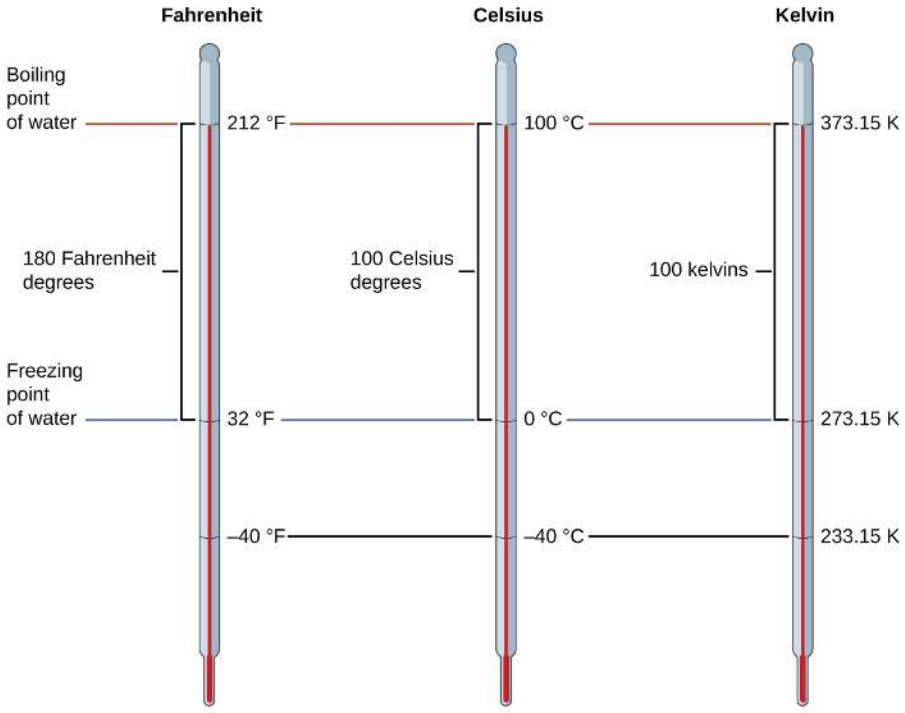


Figure **5.1.1.1**: The Fahrenheit, Celsius, and kelvin temperature scales are compared.

Although the kelvin (absolute) temperature scale is the official SI temperature scale, Celsius is commonly used in many scientific contexts and is the scale of choice for nonscience contexts in almost all areas of the world. Very few countries (the U.S. and its territories, the Bahamas, Belize, Cayman Islands, and Palau) still use Fahrenheit for weather, medicine, and cooking.

✔ Example 5.1.1.4: Conversion from Celsius

Normal body temperature has been commonly accepted as 37.0 °C (although it varies depending on time of day and method of measurement, as well as among individuals). What is this temperature on the kelvin scale and on the Fahrenheit scale?

Solution

$$K = {}^\circ C + 273.15 = 37.0 + 273.2 = 310.2 K$$

$${}^\circ F = \frac{9}{5}{}^\circ C + 32.0 = \left(\frac{9}{5} \times 37.0\right) + 32.0 = 66.6 + 32.0 = 98.6{}^\circ F$$

? Exercise 5.1.1.1

Convert 80.92 °C to K and °F.

Answer

354.07 K, 177.7 °F

✔ Example 5.1.1.5: Conversion from Fahrenheit

Baking a ready-made pizza calls for an oven temperature of 450 °F. If you are in Europe, and your oven thermometer uses the Celsius scale, what is the setting? What is the kelvin temperature?

Solution

$${}^\circ C = \frac{5}{9}({}^\circ F - 32) = \frac{5}{9}(450 - 32) = \frac{5}{9} \times 418 = 232{}^\circ C \longrightarrow \text{ set oven to } 230{}^\circ C$$
$$\text{(two significant figures}$$

$$K = {}^\circ C + 273.15 = \frac{5}{9}\,({}^\circ F - 32) = \frac{5}{9}(450 - 32) + 273.15 = 505.4 K \longrightarrow 5.1 \times 10^2 K$$

Exercise 5.1.1.1

Convert 50 °F to °C and K.

Answer

10 °C, 280 K

5.1.1.3: Footnotes

- 2 Strictly speaking, the ounce and pound are units of weight, *W* (a force equal to the product of mass and gravitational acceleration, *W* = *mg*). The conversion relations in this table are commonly used to equate masses and weight assuming a nominal value for *g* at the surface of the earth.

This page titled 5.1.1: Mathematical Treatment of Measurement Results is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.6: Mathematical Treatment of Measurement Results** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

5.2: Measurement Uncertainty, Accuracy, and Precision

Learning Objectives

By the end of this section, you will be able to:

- Define accuracy and precision
- Distinguish exact and uncertain numbers
- Correctly represent uncertainty in quantities using significant figures
- Apply proper rounding rules to computed quantities

Counting is the only type of measurement that is free from uncertainty, provided the number of objects being counted does not change while the counting process is underway. The result of such a counting measurement is an example of an **exact number**. By counting the eggs in a carton, one can determine *exactly* how many eggs the carton contains. The numbers of defined quantities are also exact. By definition, 1 foot is exactly 12 inches, 1 inch is exactly 2.54 centimeters, and 1 gram is exactly 0.001 kilogram. Quantities derived from measurements other than counting, however, are uncertain to varying extents due to practical limitations of the measurement process used.

5.2.1: Significant Figures in Measurement

The numbers of measured quantities, unlike defined or directly counted quantities, are not exact. To measure the volume of liquid in a graduated cylinder, you should make a reading at the bottom of the meniscus, the lowest point on the curved surface of the liquid.

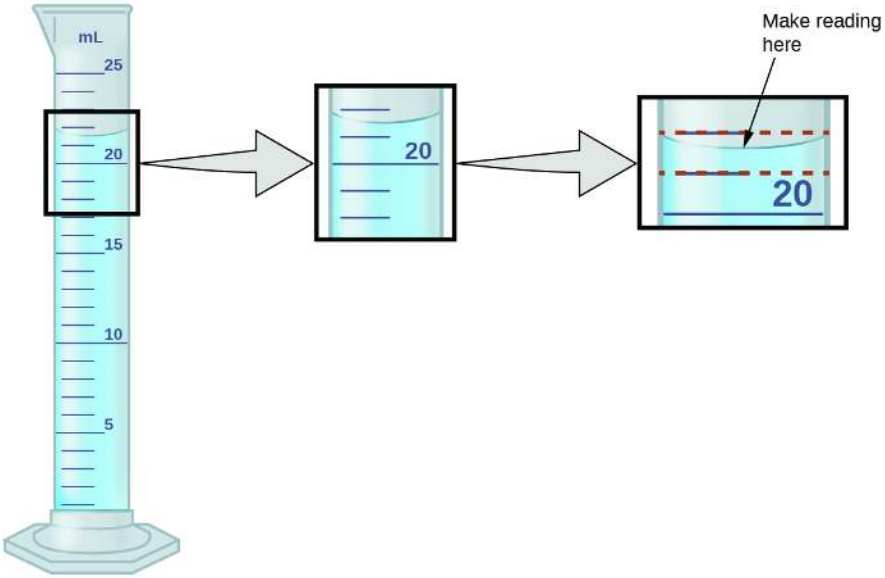
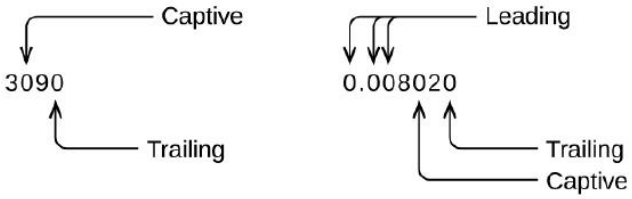


Figure 5.2.1: To measure the volume of liquid in this graduated cylinder, you must mentally subdivide the distance between the 21 and 22 mL marks into tenths of a milliliter, and then make a reading (estimate) at the bottom of the meniscus.

Refer to the illustration in Figure 5.2.1. The bottom of the meniscus in this case clearly lies between the 21 and 22 markings, meaning the liquid volume is *certainly* greater than 21 mL but less than 22 mL. The meniscus appears to be a bit closer to the 22-mL mark than to the 21-mL mark, and so a reasonable estimate of the liquid's volume would be 21.6 mL. In the number 21.6, then, the digits 2 and 1 are certain, but the 6 is an estimate. Some people might estimate the meniscus position to be equally distant from each of the markings and estimate the tenth-place digit as 5, while others may think it to be even closer to the 22-mL mark and estimate this digit to be 7. Note that it would be pointless to attempt to estimate a digit for the hundredths place, given that the tenths-place digit is uncertain. In general, numerical scales such as the one on this graduated cylinder will permit measurements to one-tenth of the smallest scale division. The scale in this case has 1-mL divisions, and so volumes may be measured to the nearest 0.1 mL.

This concept holds true for all measurements, even if you do not actively make an estimate. If you place a quarter on a standard electronic balance, you may obtain a reading of 6.72 g. The digits 6 and 7 are certain, and the 2 indicates that the mass of the quarter is likely between 6.71 and 6.73 grams. The quarter weighs *about* 6.72 grams, with a nominal uncertainty in the measurement of ± 0.01 gram. If the coin is weighed on a more sensitive balance, the mass might be 6.723 g. This means its mass lies between 6.722 and 6.724 grams, an uncertainty of 0.001 gram. Every measurement has some **uncertainty**, which depends on the device used (and the user's ability). All of the digits in a measurement, including the uncertain last digit, are called **significant figures** or **significant digits**. Note that zero may be a measured value; for example, if you stand on a scale that shows weight to the nearest pound and it shows "120," then the 1 (hundreds), 2 (tens) and 0 (ones) are all significant (measured) values.

A measurement result is properly reported when its significant digits accurately represent the certainty of the measurement process. But what if you were analyzing a reported value and trying to determine what is significant and what is not? Well, for starters, all nonzero digits are significant, and it is only zeros that require some thought. We will use the terms "leading," "trailing," and "captive" for the zeros and will consider how to deal with them.



Starting with the first nonzero digit on the left, count this digit and all remaining digits to the right. This is the number of significant figures in the measurement unless the last digit is a trailing zero lying to the left of the decimal point.

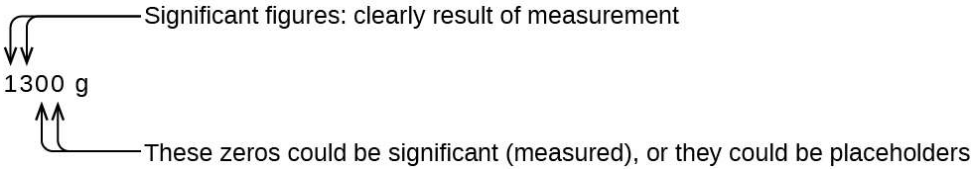


Captive zeros result from measurement and are therefore always significant. Leading zeros, however, are never significant—they merely tell us where the decimal point is located.



The leading zeros in this example are not significant. We could use exponential notation (as described in Appendix B) and express the number as 8.32407×10^{-3}; then the number 8.32407 contains all of the significant figures, and 10^{-3} locates the decimal point.

The number of significant figures is uncertain in a number that ends with a zero to the left of the decimal point location. The zeros in the measurement 1,300 grams could be significant or they could simply indicate where the decimal point is located. The ambiguity can be resolved with the use of exponential notation: 1.3×10^3 (two significant figures), 1.30×10^3 (three significant figures, if the tens place was measured), or 1.300×10^3 (four significant figures, if the ones place was also measured). In cases where only the decimal-formatted number is available, it is prudent to assume that all trailing zeros are not significant.



When determining significant figures, be sure to pay attention to reported values and think about the measurement and significant figures in terms of what is reasonable or likely when evaluating whether the value makes sense. For example, the official January 2014 census reported the resident population of the US as 317,297,725. Do you think the US population was correctly determined to the reported nine significant figures, that is, to the exact number of people? People are constantly being born, dying, or moving into or out of the country, and assumptions are made to account for the large number of people who are not actually counted. Because of these uncertainties, it might be more reasonable to expect that we know the population to within perhaps a million or so, in which case the population should be reported as $3.17\ 10^8$ people.

5.2.2: Significant Figures in Calculations

A second important principle of uncertainty is that results calculated from a measurement are at least as uncertain as the measurement itself. Take the uncertainty in measurements into account to avoid misrepresenting the uncertainty in calculated results. One way to do this is to report the result of a calculation with the correct number of significant figures, which is determined by the following three rules for **rounding** numbers:

1. When adding or subtracting numbers, round the result to the same number of decimal places as the number with the least number of decimal places (the least certain value in terms of addition and subtraction).
2. When multiplying or dividing numbers, round the result to the same number of digits as the number with the least number of significant figures (the least certain value in terms of multiplication and division).
3. If the digit to be dropped (the one immediately to the right of the digit to be retained) is less than 5, “round down” and leave the retained digit unchanged; if it is more than 5, “round up” and increase the retained digit by 1. If the dropped digit is 5, and it’s either the last digit in the number or it’s followed only by zeros, round up or down, whichever yields an even value for the retained digit. If any nonzero digits follow the dropped 5, round up. (The last part of this rule may strike you as a bit odd, but it’s based on reliable statistics and is aimed at avoiding any bias when dropping the digit “5,” since it is equally close to both possible values of the retained digit.)

The following examples illustrate the application of this rule in rounding a few different numbers to three significant figures:

- 0.028675 rounds “up” to 0.0287 (the dropped digit, 7, is greater than 5)
- 18.3384 rounds “down” to 18.3 (the dropped digit, 3, is less than 5)
- 6.8752 rounds “up” to 6.88 (the dropped digit is 5, and a nonzero digit follows it)
- 92.85 rounds “down” to 92.8 (the dropped digit is 5, and the retained digit is even)

Let’s work through these rules with a few examples.

Example 5.2.1: Rounding Numbers

Round the following to the indicated number of significant figures:

a. 31.57 (to two significant figures)
b. 8.1649 (to three significant figures)
c. 0.051065 (to four significant figures)
d. 0.90275 (to four significant figures)

Solution

a. 31.57 rounds “up” to 32 (the dropped digit is 5, and the retained digit is even)
b. 8.1649 rounds “down” to 8.16 (the dropped digit, 4, is less than 5)
c. 0.051065 rounds “down” to 0.05106 (the dropped digit is 5, and the retained digit is even)
d. 0.90275 rounds “up” to 0.9028 (the dropped digit is 5, and the retained digit is even)

Exercise 5.2.1

Round the following to the indicated number of significant figures:

a. 0.424 (to two significant figures)
b. 0.0038661 (to three significant figures)
c. 421.25 (to four significant figures)
d. 28,683.5 (to five significant figures)

Answer

a. 0.42
b. 0.00387
c. 421.2
d. 28,684

Example 5.2.2: Addition and Subtraction with Significant Figures

Rule: When adding or subtracting numbers, round the result to the same number of decimal places as the number with the fewest decimal places (i.e., the least certain value in terms of addition and subtraction).

a. Add 1.0023 g and 4.383 g.
b. Subtract 421.23 g from 486 g.

Solution

(a)

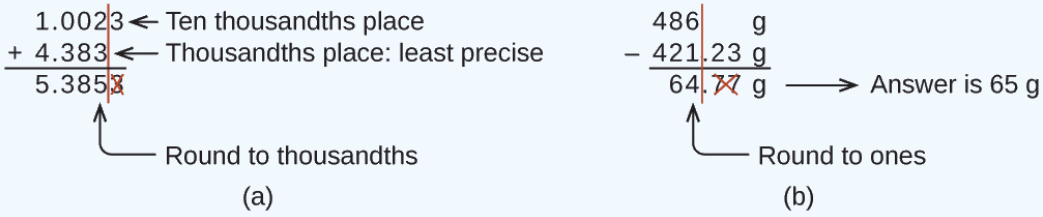
$$\begin{array}{r} 1.0023\ \text{g} \\ +\ 4.383\ \text{g} \\ \hline 5.3853\ \text{g} \end{array}$$

Answer is 5.385 g (round to the thousandths place; three decimal places)

(b)

$$\begin{array}{r} 486\ \text{g} \\ -\ 421.23\ \text{g} \\ \hline 64.77\ \text{g} \end{array}$$

Answer is 65 g (round to the ones place; no decimal places)



Exercise 5.2.2

a. Add 2.334 mL and 0.31 mL.
b. Subtract 55.8752 m from 56.533 m.

Answer

a. 2.64 mL
b. 0.658 m

Example 5.2.3: Multiplication and Division with Significant Figures

Rule: When multiplying or dividing numbers, round the result to the same number of digits as the number with the fewest significant figures (the least certain value in terms of multiplication and division).

a. Multiply 0.6238 cm by 6.6 cm.
b. Divide 421.23 g by 486 mL.

Solution

(a)

$$\underbrace{0.6238\ \text{cm}}_{\text{four significant figures}} \times \underbrace{6.6\ \text{cm}}_{\text{two significant figures}} = 4.11708\ \text{cm}^2 \rightarrow \underbrace{4.1\ \text{cm}^2}_{\text{round to two significant figures}}$$

(b)

$$\underbrace{421.23\ \text{g}}_{\text{five significant figures}} \div \underbrace{486\ \text{mL}}_{\text{three significant figures}} = 0.866728\ldots\ \text{g/mL} \rightarrow \underbrace{0.867\ \text{g/mL}}_{\text{round to three significant figures}}$$

Exercise 5.2.3

a. Multiply 2.334 cm and 0.320 cm.
b. Divide 55.8752 m by 56.53 s.

Answer

a. 0.747 cm^2
b. 0.9884 m/s

In the midst of all these technicalities, it is important to keep in mind the reason for these rules about significant figures and rounding—to correctly represent the certainty of the values reported and to ensure that a calculated result is not represented as being more certain than the least certain value used in the calculation.

Example 5.2.4: Calculation with Significant Figures

One common bathtub is 13.44 dm long, 5.920 dm wide, and 2.54 dm deep. Assume that the tub is rectangular and calculate its approximate volume in liters.

Solution

$$\begin{aligned} V &= l \times w \times d \\ &= 13.44\ \text{dm} \times 5.920\ \text{dm} \times 2.54\ \text{dm} \\ &= 202.09459\ldots\ \text{dm}^3\ \text{(value from calculator)} \\ &= 202\ \text{dm}^3\ \text{or}\ 202\ \text{L}\ \text{(answer rounded to three significant figures)} \end{aligned}$$

Exercise 5.2.4

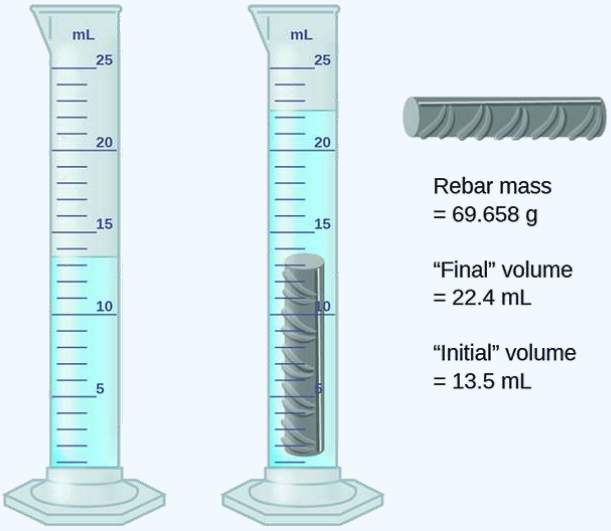
What is the density of a liquid with a mass of 31.1415 g and a volume of 30.13 cm^3?

Answer

1.034 g/mL

Example 5.2.5: Experimental Determination of Density Using Water Displacement

A piece of rebar is weighed and then submerged in a graduated cylinder partially filled with water, with results as shown.



a. Use these values to determine the density of this piece of rebar.
b. Rebar is mostly iron. Does your result in (a) support this statement? How?

Solution

The volume of the piece of rebar is equal to the volume of the water displaced:

$$\text{volume } = 22.4\,\text{mL} - 13.5\,\text{mL} = 8.9\,\text{mL} = 8.9\,\text{cm}^3$$

(rounded to the nearest 0.1 mL, per the rule for addition and subtraction)

The density is the mass-to-volume ratio:

$$\text{density } = \frac{\text{mass}}{\text{volume}} = \frac{69.658\,\text{g}}{8.9\,\text{cm}^3} = 7.8\,\text{g/cm}^3$$

(rounded to two significant figures, per the rule for multiplication and division)

The density of iron is 7.9 g/cm^3, very close to that of rebar, which lends some support to the fact that rebar is mostly iron.

? Exercise 5.2.5

An irregularly shaped piece of a shiny yellowish material is weighed and then submerged in a graduated cylinder, with results as shown.



a. Use these values to determine the density of this material.
b. Do you have any reasonable guesses as to the identity of this material? Explain your reasoning.

Answer

19 g/cm^3

It is likely gold; the right appearance for gold and very close to the known density of gold at $19.3\ \mathrm{g/cm^3}$

5.2.3: Accuracy and Precision

Scientists typically make repeated measurements of a quantity to ensure the quality of their findings and to evaluate both the precision and the accuracy of their results. Measurements are said to be precise if they yield very similar results when repeated in the same manner. A measurement is considered accurate if it yields a result that is very close to the true or accepted value. Precise values agree with each other; accurate values agree with a true value. These characterizations can be extended to other contexts, such as the results of an archery competition (Figure 5.2.2).

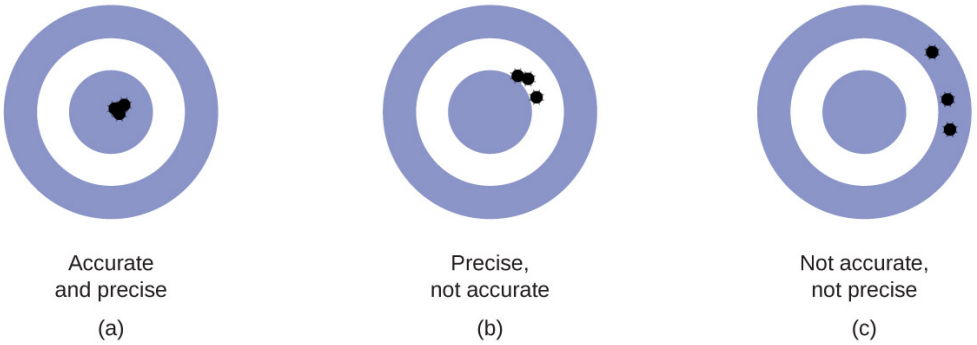


Figure 5.2.2: (a) These arrows are close to both the bull’s eye and one another, so they are both accurate and precise. (b) These arrows are close to one another but not on target, so they are precise but not accurate. (c) These arrows are neither on target nor close to one another, so they are neither accurate nor precise.

Suppose a quality control chemist at a pharmaceutical company is tasked with checking the accuracy and precision of three different machines that are meant to dispense 10 ounces (296 mL) of cough syrup into storage bottles. She proceeds to use each machine to fill five bottles and then carefully determines the actual volume dispensed, obtaining the results tabulated in Table 5.2.1.

Table 5.2.1: Volume (mL) of Cough Medicine Delivered by 10-oz (296 mL) Dispensers

Dispenser #1	Dispenser #2	Dispenser #3
283.3	298.3	296.1
284.1	294.2	295.9
283.9	296.0	296.1
284.0	297.8	296.0
284.1	293.9	296.1

Considering these results, she will report that dispenser #1 is precise (values all close to one another, within a few tenths of a milliliter) but not accurate (none of the values are close to the target value of 296 mL, each being more than 10 mL too low). Results for dispenser #2 represent improved accuracy (each volume is less than 3 mL away from 296 mL) but worse precision (volumes vary by more than 4 mL). Finally, she can report that dispenser #3 is working well, dispensing cough syrup both accurately (all volumes within 0.1 mL of the target volume) and precisely (volumes differing from each other by no more than 0.2 mL).

This page titled 5.2: Measurement Uncertainty, Accuracy, and Precision is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.5: Measurement Uncertainty, Accuracy, and Precision** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

5.3: Unit Conversions

Learning Objectives

By the end of this section, you will be able to:

- Explain the dimensional analysis (factor label) approach to mathematical calculations involving quantities
- Use dimensional analysis to carry out unit conversions for a given property and computations involving two or more properties

It is often the case that a quantity of interest may not be easy (or even possible) to measure directly but instead must be calculated from other directly measured properties and appropriate mathematical relationships. For example, consider measuring the average speed of an athlete running sprints. This is typically accomplished by measuring the *time* required for the athlete to run from the starting line to the finish line, and the *distance* between these two lines, and then computing *speed* from the equation that relates these three properties:

$$\text{speed} = \frac{\text{distance}}{\text{time}}$$

An Olympic-quality sprinter can run 100 m in approximately 10 s, corresponding to an average speed of

$$\frac{100\,\text{m}}{10\,\text{s}} = 10\,\text{m/s}$$

(For this and the next calculation, assume the trailing zeros are significant digits.) Note that this simple arithmetic involves dividing the numbers of each measured quantity to yield the number of the computed quantity (100/10 = 10) *and likewise* dividing the units of each measured quantity to yield the unit of the computed quantity (m/s = m/s). Now, consider using this same relation to predict the time required for a person running at this speed to travel a distance of 25 m. The same relation among the three properties is used, but in this case, the two quantities provided are a speed (10 m/s) and a distance (25 m). To yield the sought property, time, the equation must be rearranged appropriately:

$$\text{time} = \frac{\text{distance}}{\text{speed}}$$

The time can then be computed as:

$$\frac{25\,\text{m}}{10\,\text{m/s}} = 2.5\,\text{s}$$

Again, arithmetic on the numbers (25/10 = 2.5) was accompanied by the same arithmetic on the units (m/(m/s) = s) to yield the number and unit of the result, 2.5 s. Note that, just as for numbers, when a unit is divided by an identical unit (in this case, m/m), the result is "1"—or, as commonly phrased, the units "cancel."

These calculations are examples of a versatile mathematical approach known as **dimensional analysis** (or the **factor-label method**). Dimensional analysis is based on this premise: *the units of quantities must be subjected to the same mathematical operations as their associated numbers*. This method can be applied to computations ranging from simple unit conversions to more complex, multi-step calculations involving several different quantities.

5.3.1: Conversion Factors and Dimensional Analysis

A ratio of two equivalent quantities expressed with different measurement units can be used as a **unit conversion factor**. For example, the lengths of 2.54 cm and 1 in. are equivalent (by definition), and so a unit conversion factor may be derived from the ratio,

$$\frac{2.54\,\text{cm}}{1\,\text{in.}}\,(2.54\,\text{cm} = 1\,\text{in.}) \text{ or } 2.54\frac{\text{cm}}{\text{in.}}$$

Several other commonly used conversion factors are given in Example **5.3.1**.

Example **5.3.1**: Common Conversion Factors

Length	Volume	Mass
1 m = 1.0936 yd	1 L = 1.0567 qt	1 kg = 2.2046 lb
1 in. = 2.54 cm (exact)	1 qt = 0.94635 L	1 lb = 453.59 g
1 km = 0.62137 mi	1 ft^3 = 28.317 L	1 (avoirdupois) oz = 28.349 g
1 mi = 1609.3 m	1 tbsp = 14.787 mL	1 (troy) oz = 31.103 g

When a quantity (such as distance in inches) is multiplied by an appropriate unit conversion factor, the quantity is converted to an equivalent value with different units (such as distance in centimeters). For example, a basketball player's vertical jump of 34 inches can be converted to centimeters by:

$$34 \cancel{\text{in.}} \times \frac{2.54\,\text{cm}}{1\,\cancel{\text{in.}}} = 86\,\text{cm}$$

Since this simple arithmetic involves *quantities*, the premise of dimensional analysis requires that we multiply both *numbers and units*. The numbers of these two quantities are multiplied to yield the number of the product quantity, 86, whereas the units are multiplied to yield . Just as for numbers, a ratio of identical units is also numerically equal to one, and the unit product thus simplifies to *cm*. (When identical units divide to yield a factor of 1, they are said to "cancel.") Dimensional analysis may be used to confirm the proper application of unit conversion factors as demonstrated in the following example.

Example 5.3.1: Using a Unit Conversion Factor

The mass of a competition frisbee is 125 g. Convert its mass to ounces using the unit conversion factor derived from the relationship 1 oz = 28.349 g (Example **5.3.1**).

Solution

Given the conversion factor, the mass in ounces may be derived using an equation similar to the one used for converting length from inches to centimeters.

$$x\,oz = 125g \times \text{ unit conversion factor}$$

The unit conversion factor may be represented as:

$$\frac{1\,\text{oz}}{28.349\,\text{g}} \text{ and } \frac{28.349\,\text{g}}{1\,\text{oz}}$$

The correct unit conversion factor is the ratio that cancels the units of grams and leaves ounces.

$$\begin{aligned} x\,\text{oz} &= 125\,\text{g} \times \frac{1\,\text{oz}}{28.349\,\text{g}} \\ &= \left(\frac{125}{28.349}\right)\,\text{oz} \\ &= 4.41\,\text{oz (three significant figures)} \end{aligned}$$

Exercise 5.3.1

Convert a volume of 9.345 qt to liters.

Answer

8.844 L

Beyond simple unit conversions, the factor-label method can be used to solve more complex problems involving computations. Regardless of the details, the basic approach is the same—all the *factors* involved in the calculation must be appropriately oriented

to ensure that their *labels* (units) will appropriately cancel and/or combine to yield the desired unit in the result. As your study of chemistry continues, you will encounter many opportunities to apply this approach.

Example 5.3.2: Computing Quantities from Measurement Results and Known Mathematical Relations

What is the density of common antifreeze in units of g/mL? A 4.00-qt sample of the antifreeze weighs 9.26 lb.

Solution

Since $\text{density} = \frac{\text{mass}}{\text{volume}}$, we need to divide the mass in grams by the volume in milliliters. In general: the number of units of B = the number of units of A × unit conversion factor. The necessary conversion factors are given in Example 5.3.1: 1 lb = 453.59 g; 1 L = 1.0567 qt; 1 L = 1,000 mL. Mass may be converted from pounds to grams as follows:

$$9.26 \cancel{\text{lb}} \times \left(\frac{453.59\,\text{g}}{1\,\cancel{\text{lb}}} \right) = 4.20 \times 10^3\,\text{g}$$

Volume may be converted from quarts to milliliters via two steps:

Step 1: Convert quarts to liters.

$$4.00\,\cancel{\text{qt}} \times \left(\frac{1\,\text{L}}{1.0567\,\cancel{\text{qt}}} \right) = 3.78\,\text{L}$$

Step 2: Convert liters to milliliters.

$$3.78\,\cancel{\text{L}} \times \left(\frac{1000\,\text{mL}}{1\,\cancel{\text{L}}} \right) = 3.78 \times 10^3\,\text{mL}$$

Then,

$$\text{density} = \frac{4.20 \times 10^3\,\text{g}}{3.78 \times 10^3\,\text{mL}} = 1.11\,\text{g/mL}$$

Alternatively, the calculation could be set up in a way that uses three unit conversion factors sequentially as follows:

$$\frac{9.26\,\cancel{\text{lb}}}{4.00\,\cancel{\text{qt}}} \times \frac{453.59\,\text{g}}{1\,\cancel{\text{lb}}} \times \frac{1.0567\,\cancel{\text{qt}}}{1\,\cancel{\text{L}}} \times \frac{1\,\cancel{\text{L}}}{1000\,\text{mL}} = 1.11\,\text{g/mL}$$

Exercise 5.3.2

What is the volume in liters of 1.000 oz, given that 1 L = 1.0567 qt and 1 qt = 32 oz (exactly)?

Answer

2.956×10^{-2} L

Example 5.3.3: Computing Quantities from Measurement Results and Known Mathematical Relations

While being driven from Philadelphia to Atlanta, a distance of about 1250 km, a 2014 Lamborghini Aventador Roadster uses 213 L gasoline.

a. What (average) fuel economy, in miles per gallon, did the Roadster get during this trip?
b. If gasoline costs $3.80 per gallon, what was the fuel cost for this trip?

Solution

(a) First convert distance from kilometers to miles:

$$1250\ \cancel{\text{km}} \times \frac{0.62137\ \text{mi}}{1\ \cancel{\text{km}}} = 777\ \text{mi}$$

and then convert volume from liters to gallons:

$$213\ \cancel{\text{L}} \times \frac{1.0567\ \cancel{\text{qt}}}{1\ \cancel{\text{L}}} \times \frac{1\ \text{gal}}{4\ \cancel{\text{qt}}} = 56.3\ \text{gal}$$

Finally,

$$\text{(average) mileage} = \frac{777\ \text{mi}}{56.3\ \text{gal}} = 13.8\ \text{miles / gallon} = 13.8, \text{mpg}$$

Alternatively, the calculation could be set up in a way that uses all the conversion factors sequentially, as follows:

$$\frac{1250\ \cancel{\text{km}}}{213\ \cancel{\text{L}}} \times \frac{0.62137\ \text{mi}}{1\ \cancel{\text{km}}} \times \frac{1\ \cancel{\text{L}}}{1.0567\ \cancel{\text{qt}}} \times \frac{4\ \cancel{\text{qt}}}{1\ \text{gal}} = 13.8\ \text{mpg}$$

(b) Using the previously calculated volume in gallons, we find:

$$56.3\ \cancel{\text{gal}} \times \frac{\$3.80}{1\ \cancel{\text{gal}}} = \$214$$

? Exercise 5.3.3

A Toyota Prius Hybrid uses 59.7 L gasoline to drive from San Francisco to Seattle, a distance of 1300 km (two significant digits).

a. What (average) fuel economy, in miles per gallon, did the Prius get during this trip?
b. If gasoline costs $3.90 per gallon, what was the fuel cost for this trip?

Answer

a. 51 mpg
b. $62

5.3.2: Conversion of Temperature Units

We use the word **temperature** to refer to the hotness or coldness of a substance. One way we measure a change in temperature is to use the fact that most substances expand when their temperature increases and contract when their temperature decreases. The liquid in a common glass thermometer changes its volume as the temperature changes, and the position of the trapped liquid's surface along a printed scale may be used as a measure of temperature.

Temperature scales are defined relative to selected reference temperatures: Two of the most commonly used are the freezing and boiling temperatures of water at a specified atmospheric pressure. On the Celsius scale, 0 °C is defined as the freezing temperature of water and 100 °C as the boiling temperature of water. The space between the two temperatures is divided into 100 equal intervals, which we call degrees. On the **Fahrenheit** scale, the freezing point of water is defined as 32 °F and the boiling temperature as 212 °F. The space between these two points on a Fahrenheit thermometer is divided into 180 equal parts (degrees).

Defining the Celsius and Fahrenheit temperature scales as described in the previous paragraph results in a slightly more complex relationship between temperature values on these two scales than for different units of measure for other properties. Most measurement units for a given property are directly proportional to one another (y = mx). Using familiar length units as one example:

$$\text{length in feet} = \left(\frac{1ft}{12in.}\right) \times \text{length in inches}$$

where y = length in feet, x = length in inches, and the proportionality constant, m, is the conversion factor. The Celsius and Fahrenheit temperature scales, however, do not share a common zero point, and so the relationship between these two scales is a

linear one rather than a proportional one (y = mx + b). Consequently, converting a temperature from one of these scales into the other requires more than simple multiplication by a conversion factor, m; it also must take into account differences in the scales' zero points (b).

The linear equation relating Celsius and Fahrenheit temperatures is easily derived from the two temperatures used to define each scale. Representing the Celsius temperature as *x* and the Fahrenheit temperature as *y*, the slope, *m*, is computed to be:

$$m = \frac{\Delta y}{\Delta x} = \frac{212^\circ F - 32^\circ F}{100^\circ C - 0^\circ C} = \frac{180^\circ F}{100^\circ C} = \frac{9^\circ F}{5^\circ C}$$

The *y*-intercept of the equation, *b*, is then calculated using either of the equivalent temperature pairs, (100 °C, 212 °F) or (0 °C, 32 °F), as:

$$b = y - mx = 32^\circ F - \frac{9^\circ F}{5^\circ C} \times 0^\circ C = 32^\circ F$$

The equation relating the temperature (T) scales is then:

$$T^\circ F = \left(\frac{9^\circ F}{5^\circ C} \times T^\circ C\right) + 32^\circ F$$

An abbreviated form of this equation that omits the measurement units is:

$$T^\circ F = \left(\frac{9}{5} \times T^\circ C\right) + 32$$

Rearrangement of this equation yields the form useful for converting from Fahrenheit to Celsius:

$$T^\circ F = \left(\frac{9}{5} \times T^\circ C\right) + 32$$

As mentioned earlier in this chapter, the SI unit of temperature is the kelvin (K). Unlike the Celsius and Fahrenheit scales, the kelvin scale is an absolute temperature scale in which 0 (zero) K corresponds to the lowest temperature that can theoretically be achieved. Since the kelvin temperature scale is absolute, a degree symbol is not included in the unit abbreviation, K. The early 19th-century discovery of the relationship between a gas's volume and temperature suggested that the volume of a gas would be zero at −273.15 °C. In 1848, British physicist William Thompson, who later adopted the title of Lord Kelvin, proposed an absolute temperature scale based on this concept (further treatment of this topic is provided in this text's chapter on gases).

The freezing temperature of water on this scale is 273.15 K and its boiling temperature is 373.15 K. Notice the numerical difference in these two reference temperatures is 100, the same as for the Celsius scale, and so the linear relation between these two temperature scales will exhibit a slope of . Following the same approach, the equations for converting between the kelvin and Celsius temperature scales are derived to be:

$$T_K = T^\circ C + 273.15$$
$$T^{\circ C} = T_K - 273.15$$

The 273.15 in these equations has been determined experimentally, so it is not exact. Figure 5.3.1: shows the relationship among the three temperature scales.

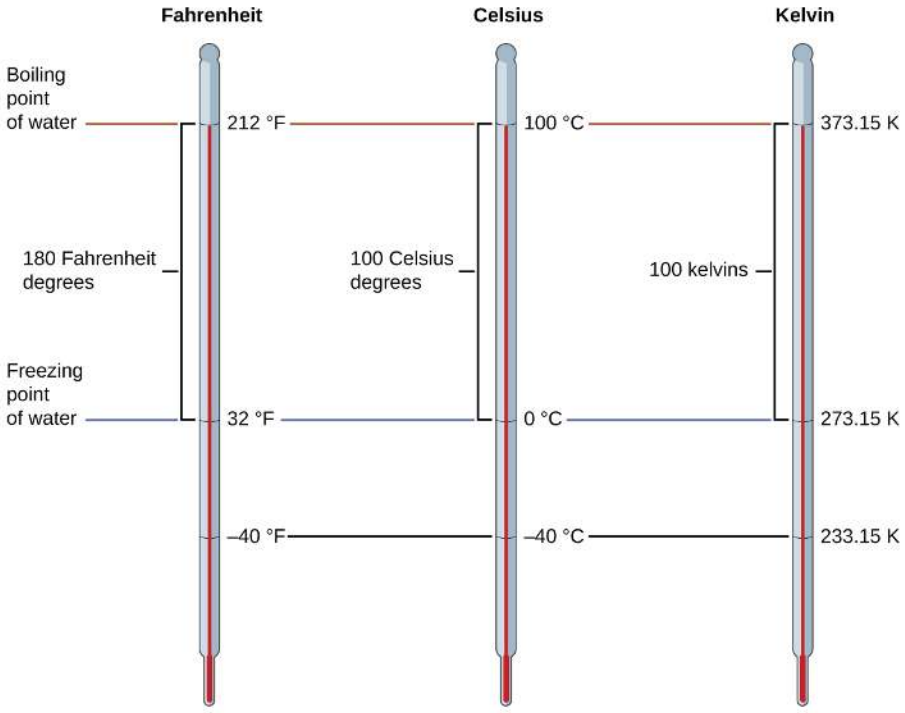


Figure **5.3.1**: The Fahrenheit, Celsius, and kelvin temperature scales are compared.

Although the kelvin (absolute) temperature scale is the official SI temperature scale, Celsius is commonly used in many scientific contexts and is the scale of choice for nonscience contexts in almost all areas of the world. Very few countries (the U.S. and its territories, the Bahamas, Belize, Cayman Islands, and Palau) still use Fahrenheit for weather, medicine, and cooking.

✔ Example 5.3.4: Conversion from Celsius

Normal body temperature has been commonly accepted as 37.0 °C (although it varies depending on time of day and method of measurement, as well as among individuals). What is this temperature on the kelvin scale and on the Fahrenheit scale?

Solution

$$K = {}^\circ C + 273.15 = 37.0 + 273.2 = 310.2 K$$

$${}^\circ F = \frac{9}{5}{}^\circ C + 32.0 = \left(\frac{9}{5} \times 37.0\right) + 32.0 = 66.6 + 32.0 = 98.6{}^\circ F$$

? Exercise 5.3.1

Convert 80.92 °C to K and °F.

Answer

354.07 K, 177.7 °F

✔ Example 5.3.5: Conversion from Fahrenheit

Baking a ready-made pizza calls for an oven temperature of 450 °F. If you are in Europe, and your oven thermometer uses the Celsius scale, what is the setting? What is the kelvin temperature?

Solution

$${}^\circ C = \frac{5}{9}({}^\circ F - 32) = \frac{5}{9}(450 - 32) = \frac{5}{9} \times 418 = 232{}^\circ C \longrightarrow \text{ set oven to } 230{}^\circ C$$
$$\text{(two significant figures}$$

$$K = {}^\circ C + 273.15 = \frac{5}{9}\,({}^\circ F - 32) = \frac{5}{9}(450 - 32) + 273.15 = 505.4 K \longrightarrow 5.1 \times 10^2 K$$

Exercise 5.3.1

Convert 50 °F to °C and K.

Answer

10 °C, 280 K

5.3.3: Footnotes

- 2 Strictly speaking, the ounce and pound are units of weight, *W* (a force equal to the product of mass and gravitational acceleration, *W* = *mg*). The conversion relations in this table are commonly used to equate masses and weight assuming a nominal value for *g* at the surface of the earth.

This page titled 5.3: Unit Conversions is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **1.6: Mathematical Treatment of Measurement Results** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

5.4: Health Connections- Dosage Calculations

Learning Objectives

- Calculate drug dosages using conversion factors.

To Your Health: Dosages

A medicine can be more harmful than helpful if it is not taken in the proper dosage. A dosage (or dose) is the specific amount of a medicine that is known to be therapeutic for an ailment in a patient of a certain size. Dosages of the active ingredient in medications are usually described by units of mass, typically grams or milligrams, and generally are equated with a number of capsules or teaspoonfuls to be swallowed or injected. The amount of the active ingredient in a medicine is carefully controlled so that the proper number of pills or spoonfuls contains the proper dose.

Most drugs must be taken in just the right amount. If too little is taken, the desired effects will not occur (or will not occur fast enough for comfort); if too much is taken, there may be potential side effects that are worse than the original ailment. Some drugs are available in multiple dosages. For example, tablets of the medication levothyroxine sodium, a synthetic thyroid hormone for those suffering from decreased thyroid gland function, are available in 11 different doses, ranging from 25 micrograms (µg) to 300 µg. It is a doctor's responsibility to prescribe the correct dosage for a patient, and it is a pharmacist's responsibility to provide the patient with the correct medicine at the dosage prescribed. Thus, proper quantities—which are expressed using numbers and their associated units—are crucial for keeping us healthy.

Effects are dose-dependent

Chemicals are the most common things for which doses are measured, but there are others, such as radiation exposure. For humans, most doses of micronutrients and medications are measured in milligrams (mg), but some are measured in micrograms because of their potency. Nonmedicinal poisons span the measurement scale; some poisons are so dangerous that a single microgram of it could be deadly, whereas other substances take much more. For example, even water is toxic when consumed in large enough quantities.

Dosage (the size of each dose) determines the strength and duration of the health benefits of nutrients, and also of the therapeutic effects of medical treatments. Dosage also determines the severity of adverse effects of treatments and toxins.

Duration of exposure, that is, the period of time over which the dose was received (all at once or gradually) also determines its effects (the body may build tolerance to gradual exposure to a drug, while a large immediate dose could be deadly).

The route by which a dose is exposed to, may affect the outcome, because some medications have different effects depending on whether they are inhaled, ingested, taken transdermally, injected, or inserted.

The dosage, route, concentration, and division over time may all be critical considerations in the administering of drugs, or in responding to exposure to a toxin. In nutrition, the route is usually a given, as nutrients are generally eaten; while dosage and the frequency of ingestion of nutrients are very important variables in preventing disease and promoting overall health.

Calculation of dose

Calculating drug dosages for humans based on the doses used in animal studies can be based on weight (e.g., mg/kg) or surface area (e.g., mg/m^2) based on weight. Drug dosage calculation is required if the physician's order is different from what is available.

Example 5.4.1

a. A physician ordered 100 mg of Demerol. Demerol is available as 50 mg per tablet. How many tablets should the nurse administer?

b. The doctor's order is 1.2 g of Folic Acid. Folic Acid is available as 800 mg per tablet. How many tablets should be taken?

Solution

a. We start with the given, 100 mg. We want to change the unit from *mg* to *tablets*. There are 50 mg in 1 tablet (Remember that *per* tablet means *one* tablet. From this relationship, we can construct the conversion factor. We use the conversion factor that

will cancel out the original unit, *mg*, and introduce the unit we are converting to, which is *tablet*.

$$100 \cancel{\text{mg}} \times \frac{1 \text{ tablet}}{50 \cancel{\text{mg}}} = 2 \text{ tablets}$$

Hence, the nurse should administer 2 tablets.

b. We start with the given, 1.2 g and we want to change *grams* to number of *tablets*. First, we convert *1.2 g* to *mg* and then convert *mg to tablets*. We need a conversion factor for each step.

$$1.2 \cancel{\text{g}} \times \frac{1{,}000 \cancel{\text{mg}}}{1 \cancel{\text{g}}} \times \frac{1 \text{ tablet}}{800 \cancel{\text{mg}}} = 1.5 \text{ tablets}$$

Hence, 1.5 tablets should be taken.

? Exercise 5.4.1

Calculate each of the following.

a. The physician ordered 20 mg of Valium. Valium is available as 10 mg per tablet. How many tablets should the nurse administer?
b. The doctor's order is 1 g of Calcium. What is on hand is Calcium as 500 mg per tablet. How many tablets should be taken?

Answer a

Start with 20 mg of Valium. For the conversion factor, we know that 10 mg Valium = 1 tablet

$$20 \cancel{\text{mg}} \times \frac{1 \text{ tablet}}{10 \cancel{\text{mg}}} = 2 \text{ tablets}$$

Answer b

Start with 1 g (1000 mg) of Calcium. For the conversion factor, we know that 500 mg Calcium = 1 tablet

$$1000 \cancel{\text{mg}} \times \frac{1 \text{ tablet}}{500 \cancel{\text{mg}}} = 2 \text{ tablets}$$

Drug Dosage Calculation based on Body Weight. Many drugs (especially in children) are dosed according to body weight (mg/kg). These calculations are carried in 3-step conversions. The first step is to convert the body weight from *pounds (lbs)* to *kg*. The second step is to convert *kg* to *mg* (the total *mg dose* calculated based on body weight). And, finally, the *mg dose* is converted to the number of *tablets*. (as in Example 1.8.1).

✓ Example 5.4.2

a. Demerol is ordered 1.5mg/kg for a patient that is 220 lbs. Demerol is available as 50 mg per tablet. How many tablets should the nurse administer?
b. A doctor prescribes amoxicillin 30mg/kg to a child weighing 73.5 lbs. Amoxicillin is available as 500 mg tablets. How many tablets should the nurse administer?

Solution

a. We start with the given, 220 *lbs*. We want to change the unit from *lbs* to *kg*, and then, from *kg* to *total dose (mg)* and then *the mg dose to tablets*. The first conversion factor will cancel out the original unit, *lbs*, and introduce the unit we are converting to, which is *kg*. The second conversion factor will cancel out *kg*, and introduce the unit of the *dose* (usually *mg*) and then *mg* to *tablet*.

$$220 \cancel{\text{lbs}} \times \frac{1 \cancel{\text{kg}}}{2.2 \cancel{\text{lbs}}} \times \frac{1.5 \cancel{\text{mg}}}{1 \cancel{\text{kg}}} \times \frac{1 \text{ tablet}}{50 \cancel{\text{mg}}} = 3 \text{ tablets}$$

Hence, the nurse administers 3 tablets.

b. Start with the given, 73.5 *lbs*. We want to change the unit from *lbs* to *kg*, and then, from *kg* to total dose (*mg*) and then *mg* to *tablets*. The first conversion factor will cancel out the original unit, *lbs*, and convert to *kg*. The second conversion factor will cancel out *kg*, and convert to the total *mg dose* and the final conversion will cancel *mg* to introduce the final unit, *tablet*.

$$73.5 \cancel{\text{ lbs}} \times \frac{1 \cancel{\text{ kg}}}{2.2 \cancel{\text{ lbs}}} \times \frac{30 \cancel{\text{ mg}}}{1 \cancel{\text{ kg}}} \times \frac{1 \text{ tablet}}{500 \cancel{\text{ mg}}} = 2 \text{ tablets}$$

Hence, the nurse administers 2 tablets.

Exercise 5.4.2

Calculate each of the following.

a. Vancomycin is ordered 15mg/kg for a patient that is 110 lbs. Vancomycin is available as 250 mg per capsule. How many capsules should the nurse administer? (ans. 3 capsules)
b. A doctor prescribes ampicillin 40mg/kg to a patient weighing 55 lbs. Ampicillin is available as 500 mg tablets. How many tablets should the nurse administer? (ans. 2 tablets)

Answer a

$$110 \cancel{\text{ lbs}} \times \frac{1 \cancel{\text{ kg}}}{2.2 \cancel{\text{ lbs}}} \times \frac{15 \cancel{\text{ mg}}}{1 \cancel{\text{ kg}}} \times \frac{1 \text{ tablet}}{250 \cancel{\text{ mg}}} = 3 \text{ tablets}$$

Answer b

$$55 \cancel{\text{ lbs}} \times \frac{1 \cancel{\text{ kg}}}{2.2 \cancel{\text{ lbs}}} \times \frac{40 \cancel{\text{ mg}}}{1 \cancel{\text{ kg}}} \times \frac{1 \text{ tablet}}{500 \cancel{\text{ mg}}} = 2 \text{ tablets}$$

References

1. The Use of Body Surface Area as a Criterion of Drug Dosage in Cancer Chemotherapy(opens in new window) [cancerres.aacrjournals.org] "The Use of Body Surface Area as a Criterion of Drug Dosage in Cancer Chemotherapy" D Pinkel. Cancer Research 1958

Contributors and Attributions

- Wikipedia
- Leticia Colmenares (UH-WCC)

This page titled 5.4: Health Connections- Dosage Calculations is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Anonymous via source content that was edited to the style and standards of the LibreTexts platform.

- **1.8: Dosage Calculations** by Anonymous is licensed CC BY-SA 4.0. Original source: https://2012books.lardbucket.org/books/introduction-to-chemistry-general-organic-and-biological.

5.5: Case Study- Precision in Pediatric Care – The Imperative of Unit Conversion

Introduction: The meticulous practice of unit conversion is a daily reality for healthcare professionals. It is especially critical in pediatric nursing, where dosages must be tailored to the smallest patients with the utmost accuracy.

Scenario: Nurse Emily starts her shift in the pediatric ward of Mercy General Hospital with a critical task: administering a new medication to Sophie, a six-year-old with a congenital heart condition. The medication, which is vital to Sophie's recovery, is prescribed in milligrams, but the stock available in the hospital pharmacy is measured in micrograms. It's Emily's responsibility to ensure that Sophie receives the exact dosage her delicate condition requires.

Personalized Unit Conversion Example: The prescription specifies 2 mg, and Emily must convert this to the appropriate number of micrograms. With the knowledge that one milligram is equivalent to 1,000 micrograms, she multiplies: $2\,\text{mg} \times 1{,}000\ \mu\text{gmg} = 2{,}000\ \mu\text{g}2\text{mg} \times 1{,}000\text{mg}\mu\text{g} = 2{,}000\mu\text{g}$. Now, Emily can confidently prepare a 2,000 microgram dose for Sophie, ensuring the precision required for her young patient's well-being.

Case Study Questions:

1. **Provide an example of a unit conversion for medication dosages.**
2. **Why is accurate unit conversion crucial in healthcare?**

Hands-On Classroom Activities:

1. **Dosage Calculation Stations:** In the "Dosage Calculation Stations" exercise, students will move through a series of stations where they will be challenged to practice the conversion of medication dosages from one unit to another. This activity is structured to enhance their proficiency in calculating and converting dosages accurately, a critical skill in ensuring patient safety and effective treatment administration.

Conclusion: In this intimate glimpse into the pediatric ward, Nurse Emily's role transcends mere calculation; it's about safeguarding a child's life through precision and attention to detail. The act of converting units becomes a profound demonstration of the care and expertise that healthcare practitioners like Emily provide. This case study serves as a testament to the critical importance of exact unit conversions in the healthcare profession, where they serve as the foundation for safe and effective patient care.

5.5: Case Study- Precision in Pediatric Care – The Imperative of Unit Conversion is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

5.E: Exercises

Multiple choice

1. How many inches are in 5.00 cm?
    a. 1.97 in
    b. 2.54 in
    c. 5.00 in
    d. 12.7 in
2. How many ounces are in 10.0 g?
    a. 0.353oz
    b. 10.0 oz
    c. 35.3 oz
    d. 353 oz
3. What is 25 °C in degrees Fahrenheit?
    a. −3.9 °F
    b. 25 °F
    c. 51 °F
    d. 77 °F
4. How many miles are in a 5.0 km race?
    a. 1.6 mi
    b. 3.1 mi
    c. 8.0 mi
    d. 5.0×10^3 mi
5. An aspirin tablet contains 325 mg acetylsalicylic acid. If a patient ingests four tables, what mass (in grams) of acetylsalicylic acid has been ingested?
    a. 0.0813 g
    b. 0.325 g
    c. 1.30 g
    d. 130. g
6. The diameter of a red blood cell is about 3.0 × 10−4 in. What is its diameter in centimeters?
    a. 1.2×10^{-4} cm
    b. 1.5×10^{-4} cm
    c. 3.0×10^{-4} cm
    d. 7.6×10^{-4} cm
7. How many in^2 are in 2.00 ft^2?
    a. 0.00694 in^2
    b. 24 in^2
    c. 144 in^2
    d. 288 in^2
8. An iron block has a mass of 197 g and a volume of 25.0 cm^3. Calculate the density of iron.
    a. 0.127 g/cm^3
    b. 7.88 g/cm^3
    c. 25.0 g/cm^3
    d. 4930 g/cm^3
9. A copper block has a mass of 10.0 g. When placed in a graduated cylinder holding water, the volume increased by 1.12 cm^3. What is the density of copper?
    a. 0.112 g/cm^3

b. 8.93 g/cm^3
c. 10.0 g/cm^3
d. 11.2 g/cm^3

10. What is the mass of a 5.00 cm^3 block of lead? The density of lead is 11.3 g/cm^3.
    a. 0.0177 g
    b. 0.442 g
    c. 2.26 g
    d. 56.5 g

Easy

1. Perform the following conversions between units:
    a. 612 g to mg
    b. 8.160 m to cm
    c. 3779 µg to g
    d. 781 mL to L
2. Perform the following conversions between units:
    a. 4.18 kg to g
    b. 27.8 m to km
    c. 0.13 mL to L
    d. 1738 km to m
3. A barrel of oil is exactly 42 gal. How many liters of oil are in a barrel?
4. How many milliliters of a soft drink are contained in a 12.0 oz can?
5. A car is driving 70 mi/hr on the highway. How far will the car travel in 35 min?
6. How long will it take a car traveling 35 mi/hr to travel 112 mi?
7. Convert the temperature of scalding water, 54 °C, into degrees Fahrenheit and kelvin.
8. Convert the temperature of the coldest area in a freezer, −10 °F, to degrees Celsius and kelvin.
9. Calculate the density of aluminum if 27.6 cm^3 has a mass of 74.6 g.
10. Osmium is one of the densest elements known. What is its density if 2.72 g has a volume of 0.121 cm^3?
11. A gold coin has a mass of 31.1 g and a volume of 1.61 cm^3. Calculate the density of gold.
12. A brass key has a mass of 8.0 g. It was placed in a graduated cylinder holding water, and the volume increased by 0.94 cm^3. What is the density of brass?

Medium

1. A typical speed limit on American highways is 65 mi/hr. Convert this speed to SI unit, m/s.
2. The density of ethanol is 0.789 g/mL. What is the density of ethanol in kg/L?
3. A small wooden block has a volume of 10.0 cm^3. What is this volume in in^3?
4. The density of water at room temperature is 0.997 g/cm^3. Restate this density in SI units, kg/m^3.

Challenge

1. A student performs an experiment to determine the density of silver. She measures the mass of a block of silver to be 9.530 g. She fills a graduated cylinder with 12.10 mL of water. Upon inserting the silver block into the graduated cylinder, the water level rises to 13.01 mL. What is the density of silver in g/cm^3?

Health-Related Questions

1. Hyperlipidemia, or too much fat in the blood, can be so significant that the fat separates from the blood. Blood has a density of 0.99 g/mL. Triglycerides (fat) have a density of 7.6 lb/gallon. What is the density of triglycerides in g/mL, and will they float or sink in blood? (1 lb = 0.453592 kg, 1 gallon = 3.78541 L).
2. Humans have, on average, 5.0 L of blood. If blood has 4.9 million red blood cells per microliter (mcL), how many red blood cells are in an entire human?

3. Cholesterol can be isolated as a solid. If 141 mg of cholesterol has the volume of 134 microliters, what is the density of cholesterol in grams per cubic centimeter?
4. Pumice is a type of rock that floats on water because it has air trapping in it. It is used in personal care products and was used in medicine hundreds of years ago. If a sample of pumice has a mass of 0.560 lbs and a volume of 0.396 L by displacement, what is the density of the pumice in g/cm^3?

5.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

6: Moles

6.1: The Mole

6.2: Formula Mass

6.3: Converting between Grams and Moles

6.4: Case Study- The Mole Concept in Clinical Laboratory Analysis

6.E: Exercises

6: Moles is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

6.1: The Mole

Learning Objectives

By the end of this section, you will be able to:

- Calculate formula masses for covalent and ionic compounds
- Define the amount unit mole and the related quantity Avogadro's number Explain the relation between mass, moles, and numbers of atoms or molecules, and perform calculations deriving these quantities from one another

Many argue that modern chemical science began when scientists started exploring the quantitative as well as the qualitative aspects of chemistry. For example, Dalton's atomic theory was an attempt to explain the results of measurements that allowed him to calculate the relative masses of elements combined in various compounds. Understanding the relationship between the masses of atoms and the chemical formulas of compounds allows us to quantitatively describe the composition of substances.

6.1.1: Formula Mass

An earlier chapter of this text described the development of the atomic mass unit, the concept of average atomic masses, and the use of chemical formulas to represent the elemental makeup of substances. These ideas can be extended to calculate the formula mass of a substance by summing the average atomic masses of all the atoms represented in the substance's formula.

6.1.1.1: Formula Mass for Covalent Substances

For covalent substances, the formula represents the numbers and types of atoms composing a single molecule of the substance; therefore, the formula mass may be correctly referred to as a molecular mass. Consider chloroform ($\mathbf{CHCl_3}$), a covalent compound once used as a surgical anesthetic and now primarily used in the production of tetrafluoroethylene, the building block for the "anti-stick" polymer, Teflon. The molecular formula of chloroform indicates that a single molecule contains one carbon atom, one hydrogen atom, and three chlorine atoms. The average molecular mass of a chloroform molecule is therefore equal to the sum of the average atomic masses of these atoms. Figure **6.1.1** outlines the calculations used to derive the molecular mass of chloroform, which is 119.37 amu.

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	1	×	12.01	=	12.01
H	1	×	1.008	=	1.008
Cl	3	×	35.45	=	106.35
				Molecular mass	119.37

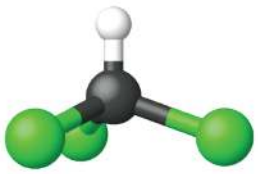


Figure **6.1.1**: The average mass of a chloroform molecule, $CHCl_3$, is 119.37 amu, which is the sum of the average atomic masses of each of its constituent atoms. The model shows the molecular structure of chloroform.

Likewise, the molecular mass of an aspirin molecule, $\mathbf{C_9H_8O_4}$, is the sum of the atomic masses of nine carbon atoms, eight hydrogen atoms, and four oxygen atoms, which amounts to 180.15 amu (Figure **6.1.2**).

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	9	×	12.01	=	108.09
H	8	×	1.008	=	8.064
O	4	×	16.00	=	64.00
				Molecular mass	180.15

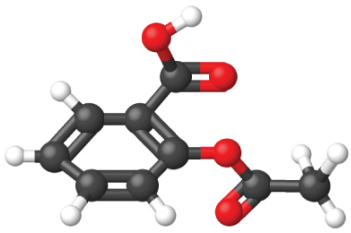


Figure **6.1.2**: The average mass of an aspirin molecule is 180.15 amu. The model shows the molecular structure of aspirin, $C_9H_8O_4$.

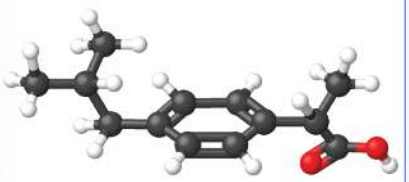
Example 6.1.1: Computing Molecular Mass for a Covalent Compound

Ibuprofen, $C_{13}H_{18}O_2$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Advil and Motrin. What is the molecular mass (amu) for this compound?

Solution

Molecules of this compound are composed of 13 carbon atoms, 18 hydrogen atoms, and 2 oxygen atoms. Following the approach described above, the average molecular mass for this compound is therefore:

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	13	×	12.01	=	156.13
H	18	×	1.008	=	18.144
O	2	×	16.00	=	32.00
				Molecular mass	206.27



Exercise 6.1.1

Acetaminophen, $C_8H_9NO_2$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Tylenol. What is the molecular mass (amu) for this compound?

Answer

151.16 amu

6.1.1.2: Formula Mass for Ionic Compounds

Ionic compounds are composed of discrete cations and anions combined in ratios to yield electrically neutral bulk matter. The formula mass for an ionic compound is calculated in the same way as the formula mass for covalent compounds: by summing the average atomic masses of all the atoms in the compound's formula. Keep in mind, however, that the formula for an ionic compound does not represent the composition of a discrete molecule, so it may not correctly be referred to as the "molecular mass."

As an example, consider sodium chloride, NaCl, the chemical name for common table salt. Sodium chloride is an ionic compound composed of sodium cations, Na^+, and chloride anions, Cl^-, combined in a 1:1 ratio. The formula mass for this compound is computed as 58.44 amu (see Figure **6.1.3**).

Element	Quantity		Average atomic mass (amu)		Subtotal
Na	1	×	22.99	=	22.99
Cl	1	×	35.45	=	35.45
				Formula mass	58.44

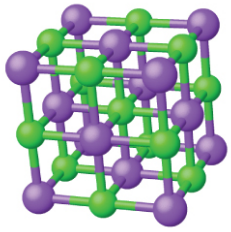


Figure **6.1.3**: Table salt, NaCl, contains an array of sodium and chloride ions combined in a 1:1 ratio. Its formula mass is 58.44 amu.

Note that the average masses of neutral sodium and chlorine atoms were used in this computation, rather than the masses for sodium cations and chlorine anions. This approach is perfectly acceptable when computing the formula mass of an ionic compound. Even though a sodium cation has a slightly smaller mass than a sodium atom (since it is missing an electron), this difference will be offset by the fact that a chloride anion is slightly more massive than a chloride atom (due to the extra electron). Moreover, the mass of an electron is negligibly small with respect to the mass of a typical atom. Even when calculating the mass of an isolated ion, the missing or additional electrons can generally be ignored, since their contribution to the overall mass is negligible, reflected only in the nonsignificant digits that will be lost when the computed mass is properly rounded. The few exceptions to this guideline are very light ions derived from elements with precisely known atomic masses.

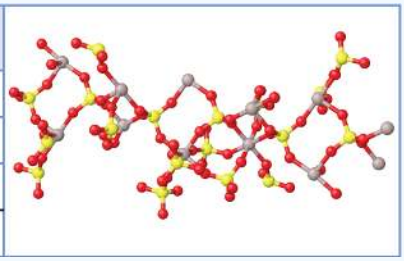
Example 6.1.2: Computing Formula Mass for an Ionic Compound

Aluminum sulfate, $Al_2(SO_4)_3$, is an ionic compound that is used in the manufacture of paper and in various water purification processes. What is the formula mass (amu) of this compound?

Solution

The formula for this compound indicates it contains Al^{3+} and SO_4^{2-} ions combined in a 2:3 ratio. For purposes of computing a formula mass, it is helpful to rewrite the formula in the simpler format, $Al_2S_3O_{12}$. Following the approach outlined above, the formula mass for this compound is calculated as follows:

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
Al	2	×	26.98	=	53.96
S	3	×	32.06	=	96.18
O	12	×	16.00	=	192.00
				Molecular mass	342.14



Exercise 6.1.2

Calcium phosphate, $Ca_3(PO_4)_2$, is an ionic compound and a common anti-caking agent added to food products. What is the formula mass (amu) of calcium phosphate?

Answer

310.18 amu

6.1.2: The Mole

The identity of a substance is defined not only by the types of atoms or ions it contains, but by the quantity of each type of atom or ion. For example, water, H_2O, and hydrogen peroxide, H_2O_2, are alike in that their respective molecules are composed of hydrogen and oxygen atoms. However, because a hydrogen peroxide molecule contains two oxygen atoms, as opposed to the water molecule, which has only one, the two substances exhibit very different properties. Today, sophisticated instruments allow the direct measurement of these defining microscopic traits; however, the same traits were originally derived from the measurement of macroscopic properties (the masses and volumes of bulk quantities of matter) using relatively simple tools (balances and volumetric glassware). This experimental approach required the introduction of a new unit for amount of substances, the *mole*, which remains indispensable in modern chemical science.

The *mole* is an amount unit similar to familiar units like pair, dozen, gross, etc. It provides a specific measure of *the number* of atoms or molecules in a sample of matter. One Latin connotation for the word “mole” is “large mass” or “bulk,” which is consistent with its use as the name for this unit. The mole provides a link between an easily measured macroscopic property, bulk mass, and an extremely important fundamental property, number of atoms, molecules, and so forth. A mole of substance is that amount in which there are $6.02214076 \times 10^{23}$.

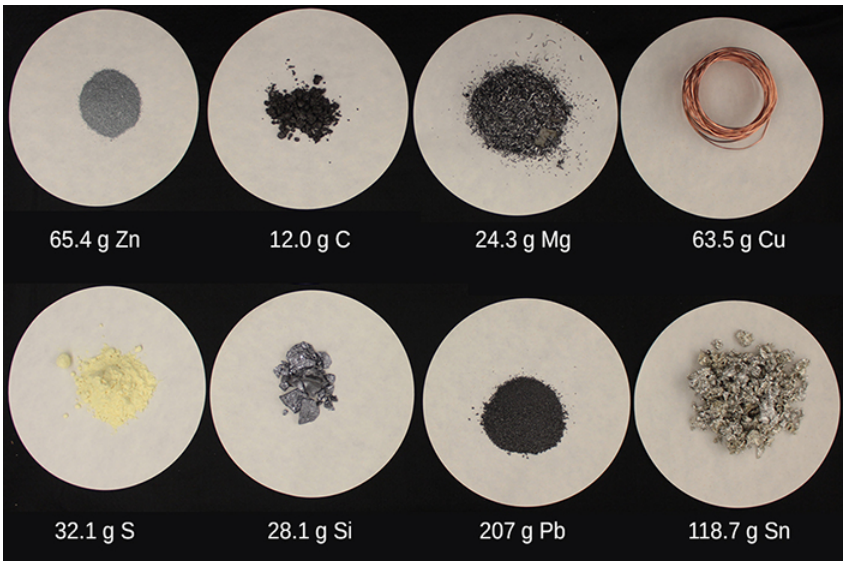


Figure **6.1.4**: Each sample contains 6.022 10^{23} atoms —1.00 mol of atoms. From left to right (top row): 65.4 g zinc, 12.0 g carbon, 24.3 g magnesium, and 63.5 g copper. From left to right (bottom row): 32.1 g sulfur, 28.1 g silicon, 207 g lead, and 118.7 g tin. (credit: modification of work by Mark Ott)

The molar mass of any substance is numerically equivalent to its atomic or formula weight in amu. Per the amu definition, a single ^{12}C atom weighs 12 amu (its atomic mass is 12 amu). A mole of ^{12}C weighs 12 g (its molar mass is 12 g/mol). This relationship holds for all elements, since their atomic masses are measured relative to that of the amu-reference substance, ^{12}C. Extending this principle, the molar mass of a compound in grams is likewise numerically equivalent to its formula mass in amu (Figure **6.1.5**).



Figure **6.1.5**: Each sample contains 6.02 10^{23} molecules or formula units—1.00 mol of the compound or element. Clock-wise from the upper left: 130.2 g of $C_8H_{17}OH$ (1-octanol, formula mass 130.2 amu), 454.4 g of HgI_2 (mercury(II) iodide, formula mass 454.4 amu), 32.0 g of CH_3OH (methanol, formula mass 32.0 amu) and 256.5 g of S_8 (sulfur, formula mass 256.5 amu). (credit: Sahar Atwa)

Element	Average Atomic Mass (amu)	Molar Mass (g/mol)	Atoms/Mole
C	12.01	12.01	6.022 10^{23}
H	1.008	1.008	6.022 10^{23}
O	16.00	16.00	6.022 10^{23}
Na	22.99	22.99	6.022 10^{23}
Cl	35.45	35.45	6.022 10^{23}

While atomic mass and molar mass are numerically equivalent, keep in mind that they are vastly different in terms of scale, as represented by the vast difference in the magnitudes of their respective units (amu versus g). To appreciate the enormity of the mole, consider a small drop of water weighing about 0.03 g (see Figure **6.1.6**). Although this represents just a tiny fraction of 1 mole of water (~18 g), it contains more water molecules than can be clearly imagined. If the molecules were distributed equally among the roughly seven billion people on earth, each person would receive more than 100 billion molecules.



Figure **6.1.6**: The number of molecules in a single droplet of water is roughly 100 billion times greater than the number of people on earth. (credit: "tanakawho"/Wikimedia commons)

Link to Learning

The mole is used in chemistry to represent 6.022 10^{23} of something, but it can be difficult to conceptualize such a large number. Watch this video and then complete the "Think" questions that follow. Explore more about the mole by reviewing the information under "Dig Deeper."

The relationships between formula mass, the mole, and Avogadro's number can be applied to compute various quantities that describe the composition of substances and compounds, as demonstrated in the next several example problems.

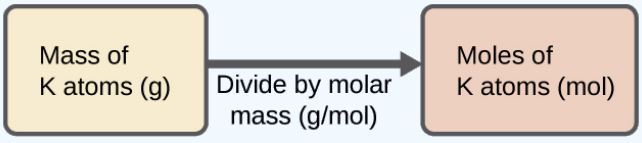
Example 6.1.3: Deriving Moles from Grams for an Element

According to nutritional guidelines from the US Department of Agriculture, the estimated average requirement for dietary potassium is 4.7 g. What is the estimated average requirement of potassium in moles?

Solution

The mass of K is provided, and the corresponding amount of K in moles is requested. Referring to the periodic table, the atomic mass of K is 39.10 amu, and so its molar mass is 39.10 g/mol. The given mass of K (4.7 g) is a bit more than one-tenth the molar mass (39.10 g), so a reasonable "ballpark" estimate of the number of moles would be slightly greater than 0.1 mol.

The molar amount of a substance may be calculated by dividing its mass (g) by its molar mass (g/mol):



The factor-label method supports this mathematical approach since the unit "g" cancels and the answer has units of "mol:"

$$4.7\ \cancel{\text{g K}}\left(\frac{\text{mol K}}{39.10\ \cancel{\text{g K}}}\right) = 0.12\,\text{mol K}$$

The calculated magnitude (0.12 mol K) is consistent with our ballpark expectation, since it is a bit greater than 0.1 mol,

Exercise 6.1.3

Beryllium is a light metal used to fabricate transparent X-ray windows for medical imaging instruments. How many moles of Be are in a thin-foil window weighing 3.24 g?

Answer

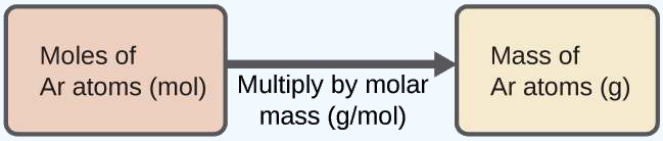
0.360 mol

Example 6.1.4: Deriving Grams from Moles for an Element

A liter of air contains 9.2 10^{-4} mol argon. What is the mass of Ar in a liter of air?

Solution

The molar amount of Ar is provided and must be used to derive the corresponding mass in grams. Since the amount of Ar is less than 1 mole, the mass will be less than the mass of 1 mole of Ar, approximately 40 g. The molar amount in question is approximately one-one thousandth (~10^{-3}) of a mole, and so the corresponding mass should be roughly one-one thousandth of the molar mass (~0.04 g):



In this case, logic dictates (and the factor-label method supports) multiplying the provided amount (mol) by the molar mass (g/mol):

$$9.2 \times 10^{-4} \cancel{\text{mol Ar}} \left(\frac{39.95 \text{ g Ar}}{\cancel{\text{mol Ar}}} \right) = 0.037 \text{ g Ar}$$

The result is in agreement with our expectations, around 0.04 g Ar.

Exercise 6.1.1

What is the mass of 2.561 mol of gold?

Answer

504.4 g

Example 6.1.5: Deriving Number of Atoms from Mass for an Element

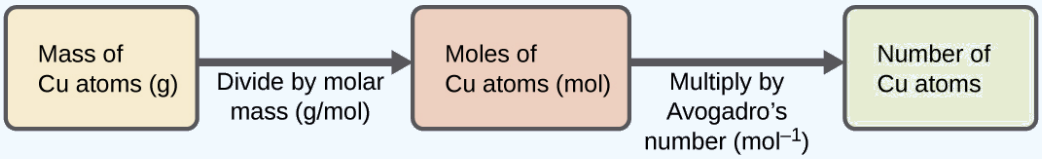
Copper is commonly used to fabricate electrical wire (Figure 6.1.7). How many copper atoms are in 5.00 g of copper wire?



Figure **6.1.7**: Copper wire is composed of many, many atoms of Cu. (credit: Emilian Robert Vicol)

Solution

The number of Cu atoms in the wire may be conveniently derived from its mass by a two-step computation: first calculating the molar amount of Cu, and then using Avogadro's number (N_A) to convert this molar amount to number of Cu atoms:



Considering that the provided sample mass (5.00 g) is a little less than one-tenth the mass of 1 mole of Cu (~64 g), a reasonable estimate for the number of atoms in the sample would be on the order of one-tenth N_A, or approximately 10^{22} Cu atoms. Carrying out the two-step computation yields:

$$5.00\ \cancel{\text{g Cu}} \left(\frac{\cancel{\text{mol Cu}}}{63.55\ \cancel{\text{g Cu}}}\right)\left(\frac{6.022 \times 10^{23}\ \text{Cu atoms}}{\cancel{\text{mol Cu}}}\right) = 4.74 \times 10^{22}\ \text{Cu atoms}$$

The factor-label method yields the desired cancellation of units, and the computed result is on the order of 10^{22} as expected.

? Exercise 6.1.5

A prospector panning for gold in a river collects 15.00 g of pure gold. How many Au atoms are in this quantity of gold?

Answer

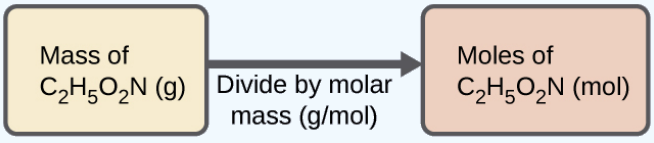
4.586×10^{22} Au atoms

✓ Example 6.1.6: Deriving Moles from Grams for a Compound

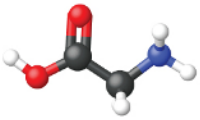
Our bodies synthesize protein from amino acids. One of these amino acids is glycine, which has the molecular formula $C_2H_5O_2N$. How many moles of glycine molecules are contained in 28.35 g of glycine?

Solution

Derive the number of moles of a compound from its mass following the same procedure used for an element in Example **6.1.3**:



The molar mass of glycine is required for this calculation, and it is computed in the same fashion as its molecular mass. One mole of glycine, $C_2H_5O_2N$, contains 2 moles of carbon, 5 moles of hydrogen, 2 moles of oxygen, and 1 mole of nitrogen:

Element	Quantity (mol element/ mol compound)		Molar mass (g/mol element)		Subtotal (g/mol compound)	
C	2	×	12.01	=	24.02	
H	5	×	1.008	=	5.040	
O	2	×	16.00	=	32.00	
N	1	×	14.007	=	14.007	
Molecular mass (g/mol compound)					75.07	

The provided mass of glycine (~28 g) is a bit more than one-third the molar mass (~75 g/mol), so the computed result is expected to be a bit greater than one-third of a mole (~0.33 mol). Dividing the compound's mass by its molar mass yields:

$$28.35 \cancel{\text{ g glycine}} \left(\frac{\text{mol glycine}}{75.07 \cancel{\text{ g glycine}}} \right) = 0.378 \text{ mol glycine}$$

This result is consistent with the rough estimate,

? Exercise 6.1.6

How many moles of sucrose, $C_{12}H_{22}O_{11}$, are in a 25-g sample of sucrose?

Answer

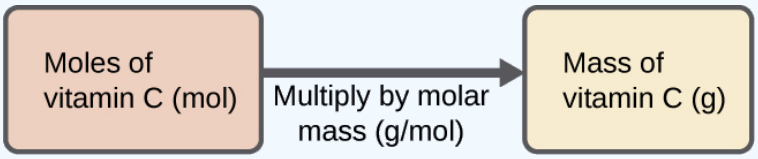
0.073 mol

✔ Example 6.1.7: Deriving Grams from Moles for a Compound

Vitamin C is a covalent compound with the molecular formula $C_6H_8O_6$. The recommended daily dietary allowance of vitamin C for children aged 4–8 years is $1.42\ 10^{-4}$ mol. What is the mass of this allowance in grams?

Solution

As for elements, the mass of a compound can be derived from its molar amount as shown:



The molar mass for this compound is computed to be 176.124 g/mol. The given number of moles is a very small fraction of a mole (~10^{-4} or one-ten thousandth); therefore, the corresponding mass is expected to be about one-ten thousandth of the molar mass (~0.02 g). Performing the calculation yields:

$$1.42 \times 10^{-4} \cancel{\text{ mol vitamin C}} \left(\frac{176.124 \text{ g vitamin C}}{\cancel{\text{mol vitamin C}}} \right) = 0.0250 \text{ g vitamin C}$$

This is consistent with the anticipated result.

? Exercise 6.1.7

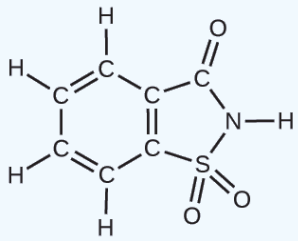
What is the mass of 0.443 mol of hydrazine, N_2H_4?

Answer

14.2 g

Example 6.1.8: Deriving the Number of Atoms and Molecules from the Mass of a Compound

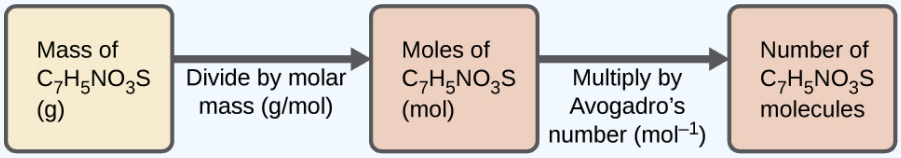
A packet of an artificial sweetener contains 40.0 mg of saccharin ($C_7H_5NO_3S$), which has the structural formula:



Given that saccharin has a molar mass of 183.18 g/mol, how many saccharin molecules are in a 40.0-mg (0.0400-g) sample of saccharin? How many carbon atoms are in the same sample?

Solution

The number of molecules in a given mass of compound is computed by first deriving the number of moles, as demonstrated in Example **6.1.6**, and then multiplying by Avogadro's number:



Using the provided mass and molar mass for saccharin yields:

$$0.0400\ \cancel{\text{g } C_7H_5NO_3S}\left(\frac{\cancel{\text{mol } C_7H_5NO_3S}}{183.18\ \cancel{\text{g } CH_5NO_3S}}\right)\left(\frac{6.022\times10^{23}\ C_7H_5NO_3S\text{ molecules}}{1\ \cancel{\text{mol } C_7H_5NO_3S}}\right)$$
$$= 1.31\times10^{20}\ C_7H_5NO_3S\text{ molecules}$$

The compound's formula shows that each molecule contains seven carbon atoms, and so the number of C atoms in the provided sample is:

$$1.31\times10^{20}\ C_7H_5NO_3S\text{ molecules}\left(\frac{7\ C\text{ atoms}}{1\ C_7H_5NO_3S\text{ molecule}}\right) = 9.17\times10^{20}\ C\text{ atoms}$$

Exercise 6.1.8

How many C_4H_{10} molecules are contained in 9.213 g of this compound? How many hydrogen atoms?

Answer

9.545×10^{22} molecules C_4H_{10}

9.545×10^{23} atoms H

How Sciences Interconnect: Counting Neurotransmitter Molecules in the Brain

The brain is the control center of the central nervous system (Figure **6.1.8**). It sends and receives signals to and from muscles and other internal organs to monitor and control their functions; it processes stimuli detected by sensory organs to guide interactions with the external world; and it houses the complex physiological processes that give rise to our intellect and emotions. The broad field of neuroscience spans all aspects of the structure and function of the central nervous system, including research on the anatomy and physiology of the brain. Great progress has been made in brain research over the past few decades, and the BRAIN Initiative, a federal initiative announced in 2013, aims to accelerate and capitalize on these

advances through the concerted efforts of various industrial, academic, and government agencies (more details available at www.whitehouse.gov/share/brain-initiative).

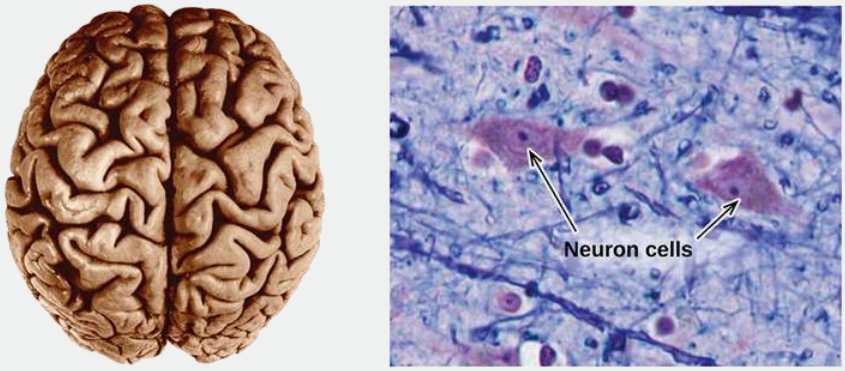


Figure **6.1.8**: (a) A typical human brain weighs about 1.5 kg and occupies a volume of roughly 1.1 L. (b) Information is transmitted in brain tissue and throughout the central nervous system by specialized cells called neurons (micrograph shows cells at 1600× magnification).

Specialized cells called neurons transmit information between different parts of the central nervous system by way of electrical and chemical signals. Chemical signaling occurs at the interface between different neurons when one of the cells releases molecules (called neurotransmitters) that diffuse across the small gap between the cells (called the synapse) and bind to the surface of the other cell. These neurotransmitter molecules are stored in small intracellular structures called vesicles that fuse to the cell membrane and then break open to release their contents when the neuron is appropriately stimulated. This process is called exocytosis (see Figure **6.1.9**). One neurotransmitter that has been very extensively studied is dopamine, $C_8H_{11}NO_2$. Dopamine is involved in various neurological processes that impact a wide variety of human behaviors. Dysfunctions in the dopamine systems of the brain underlie serious neurological diseases such as Parkinson's and schizophrenia.

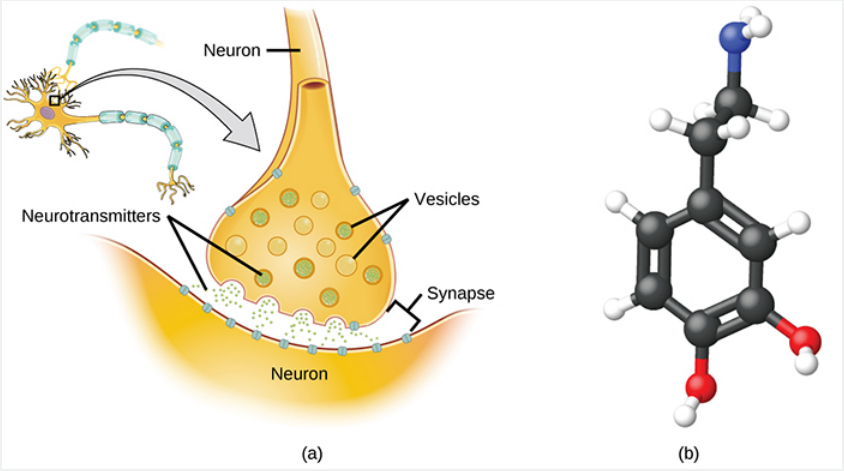


Figure **6.1.9**: (a) Chemical signals are transmitted from neurons to other cells by the release of neurotransmitter molecules into the small gaps (synapses) between the cells. (b) Dopamine, $C_8H_{11}NO_2$, is a neurotransmitter involved in a number of neurological processes.

One important aspect of the complex processes related to dopamine signaling is the number of neurotransmitter molecules released during exocytosis. Since this number is a central factor in determining neurological response (and subsequent human thought and action), it is important to know how this number changes with certain controlled stimulations, such as the administration of drugs. It is also important to understand the mechanism responsible for any changes in the number of neurotransmitter molecules released—for example, some dysfunction in exocytosis, a change in the number of vesicles in the neuron, or a change in the number of neurotransmitter molecules in each vesicle.

Significant progress has been made recently in directly measuring the number of dopamine molecules stored in individual vesicles and the amount actually released when the vesicle undergoes exocytosis. Using miniaturized probes that can

selectively detect dopamine molecules in very small amounts, scientists have determined that the vesicles of a certain type of mouse brain neuron contain an average of 30,000 dopamine molecules per vesicle (about 5×10^{-20} mol or 50 zmol). Analysis of these neurons from mice subjected to various drug therapies shows significant changes in the average number of dopamine molecules contained in individual vesicles, increasing or decreasing by up to three-fold, depending on the specific drug used. These studies also indicate that not all of the dopamine in a given vesicle is released during exocytosis, suggesting that it may be possible to regulate the fraction released using pharmaceutical therapies.

6.1.3: Footnotes

- 1Omiatek, Donna M., Amanda J. Bressler, Ann-Sofie Cans, Anne M. Andrews, Michael L. Heien, and Andrew G. Ewing. "The Real Catecholamine Content of Secretory Vesicles in the CNS Revealed by Electrochemical Cytometry." *Scientific Report* 3 (2013): 1447, accessed January 14, 2015, doi:10.1038/srep01447.

This page titled 6.1: The Mole is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **3.1: Formula Mass and the Mole Concept** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

6.2: Formula Mass

Learning Objectives

By the end of this section, you will be able to:

- Calculate formula masses for covalent and ionic compounds
- Define the amount unit mole and the related quantity Avogadro's number Explain the relation between mass, moles, and numbers of atoms or molecules, and perform calculations deriving these quantities from one another

Many argue that modern chemical science began when scientists started exploring the quantitative as well as the qualitative aspects of chemistry. For example, Dalton's atomic theory was an attempt to explain the results of measurements that allowed him to calculate the relative masses of elements combined in various compounds. Understanding the relationship between the masses of atoms and the chemical formulas of compounds allows us to quantitatively describe the composition of substances.

6.2.1: Formula Mass

An earlier chapter of this text described the development of the atomic mass unit, the concept of average atomic masses, and the use of chemical formulas to represent the elemental makeup of substances. These ideas can be extended to calculate the formula mass of a substance by summing the average atomic masses of all the atoms represented in the substance's formula.

6.2.1.1: Formula Mass for Covalent Substances

For covalent substances, the formula represents the numbers and types of atoms composing a single molecule of the substance; therefore, the formula mass may be correctly referred to as a molecular mass. Consider chloroform ($\mathbf{CHCl_3}$), a covalent compound once used as a surgical anesthetic and now primarily used in the production of tetrafluoroethylene, the building block for the "anti-stick" polymer, Teflon. The molecular formula of chloroform indicates that a single molecule contains one carbon atom, one hydrogen atom, and three chlorine atoms. The average molecular mass of a chloroform molecule is therefore equal to the sum of the average atomic masses of these atoms. Figure **6.2.1** outlines the calculations used to derive the molecular mass of chloroform, which is 119.37 amu.

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	1	×	12.01	=	12.01
H	1	×	1.008	=	1.008
Cl	3	×	35.45	=	106.35
				Molecular mass	119.37

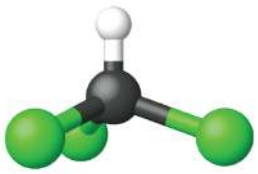


Figure **6.2.1**: The average mass of a chloroform molecule, $CHCl_3$, is 119.37 amu, which is the sum of the average atomic masses of each of its constituent atoms. The model shows the molecular structure of chloroform.

Likewise, the molecular mass of an aspirin molecule, $\mathbf{C_9H_8O_4}$, is the sum of the atomic masses of nine carbon atoms, eight hydrogen atoms, and four oxygen atoms, which amounts to 180.15 amu (Figure **6.2.2**).

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	9	×	12.01	=	108.09
H	8	×	1.008	=	8.064
O	4	×	16.00	=	64.00
				Molecular mass	180.15

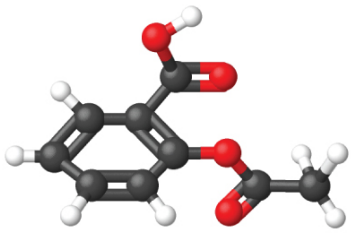


Figure **6.2.2**: The average mass of an aspirin molecule is 180.15 amu. The model shows the molecular structure of aspirin, $C_9H_8O_4$.

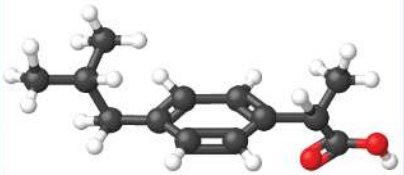
Example 6.2.1: Computing Molecular Mass for a Covalent Compound

Ibuprofen, $C_{13}H_{18}O_2$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Advil and Motrin. What is the molecular mass (amu) for this compound?

Solution

Molecules of this compound are composed of 13 carbon atoms, 18 hydrogen atoms, and 2 oxygen atoms. Following the approach described above, the average molecular mass for this compound is therefore:

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	13	×	12.01	=	156.13
H	18	×	1.008	=	18.144
O	2	×	16.00	=	32.00
				Molecular mass	206.27



Exercise 6.2.1

Acetaminophen, $C_8H_9NO_2$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Tylenol. What is the molecular mass (amu) for this compound?

Answer

151.16 amu

6.2.1.2: Formula Mass for Ionic Compounds

Ionic compounds are composed of discrete cations and anions combined in ratios to yield electrically neutral bulk matter. The formula mass for an ionic compound is calculated in the same way as the formula mass for covalent compounds: by summing the average atomic masses of all the atoms in the compound's formula. Keep in mind, however, that the formula for an ionic compound does not represent the composition of a discrete molecule, so it may not correctly be referred to as the "molecular mass."

As an example, consider sodium chloride, NaCl, the chemical name for common table salt. Sodium chloride is an ionic compound composed of sodium cations, Na^+, and chloride anions, Cl^-, combined in a 1:1 ratio. The formula mass for this compound is computed as 58.44 amu (see Figure **6.2.3**).

Element	Quantity		Average atomic mass (amu)		Subtotal
Na	1	×	22.99	=	22.99
Cl	1	×	35.45	=	35.45
				Formula mass	58.44

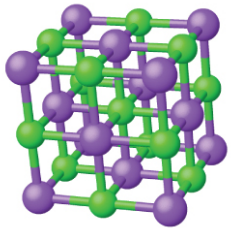


Figure **6.2.3**: Table salt, NaCl, contains an array of sodium and chloride ions combined in a 1:1 ratio. Its formula mass is 58.44 amu.

Note that the average masses of neutral sodium and chlorine atoms were used in this computation, rather than the masses for sodium cations and chlorine anions. This approach is perfectly acceptable when computing the formula mass of an ionic compound. Even though a sodium cation has a slightly smaller mass than a sodium atom (since it is missing an electron), this difference will be offset by the fact that a chloride anion is slightly more massive than a chloride atom (due to the extra electron). Moreover, the mass of an electron is negligibly small with respect to the mass of a typical atom. Even when calculating the mass of an isolated ion, the missing or additional electrons can generally be ignored, since their contribution to the overall mass is negligible, reflected only in the nonsignificant digits that will be lost when the computed mass is properly rounded. The few exceptions to this guideline are very light ions derived from elements with precisely known atomic masses.

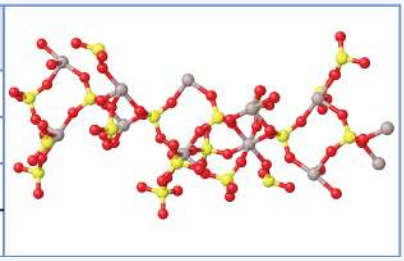
Example 6.2.2: Computing Formula Mass for an Ionic Compound

Aluminum sulfate, $Al_2(SO_4)_3$, is an ionic compound that is used in the manufacture of paper and in various water purification processes. What is the formula mass (amu) of this compound?

Solution

The formula for this compound indicates it contains Al^{3+} and SO_4^{2-} ions combined in a 2:3 ratio. For purposes of computing a formula mass, it is helpful to rewrite the formula in the simpler format, $Al_2S_3O_{12}$. Following the approach outlined above, the formula mass for this compound is calculated as follows:

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
Al	2	×	26.98	=	53.96
S	3	×	32.06	=	96.18
O	12	×	16.00	=	192.00
				Molecular mass	342.14



Exercise 6.2.2

Calcium phosphate, $Ca_3(PO_4)_2$, is an ionic compound and a common anti-caking agent added to food products. What is the formula mass (amu) of calcium phosphate?

Answer

310.18 amu

6.2.2: The Mole

The identity of a substance is defined not only by the types of atoms or ions it contains, but by the quantity of each type of atom or ion. For example, water, H_2O, and hydrogen peroxide, H_2O_2, are alike in that their respective molecules are composed of hydrogen and oxygen atoms. However, because a hydrogen peroxide molecule contains two oxygen atoms, as opposed to the water molecule, which has only one, the two substances exhibit very different properties. Today, sophisticated instruments allow the direct measurement of these defining microscopic traits; however, the same traits were originally derived from the measurement of macroscopic properties (the masses and volumes of bulk quantities of matter) using relatively simple tools (balances and volumetric glassware). This experimental approach required the introduction of a new unit for amount of substances, the *mole*, which remains indispensable in modern chemical science.

The *mole* is an amount unit similar to familiar units like pair, dozen, gross, etc. It provides a specific measure of *the number* of atoms or molecules in a sample of matter. One Latin connotation for the word “mole” is “large mass” or “bulk,” which is consistent with its use as the name for this unit. The mole provides a link between an easily measured macroscopic property, bulk mass, and an extremely important fundamental property, number of atoms, molecules, and so forth. A mole of substance is that amount in which there are $6.02214076 \times 10^{23}$.

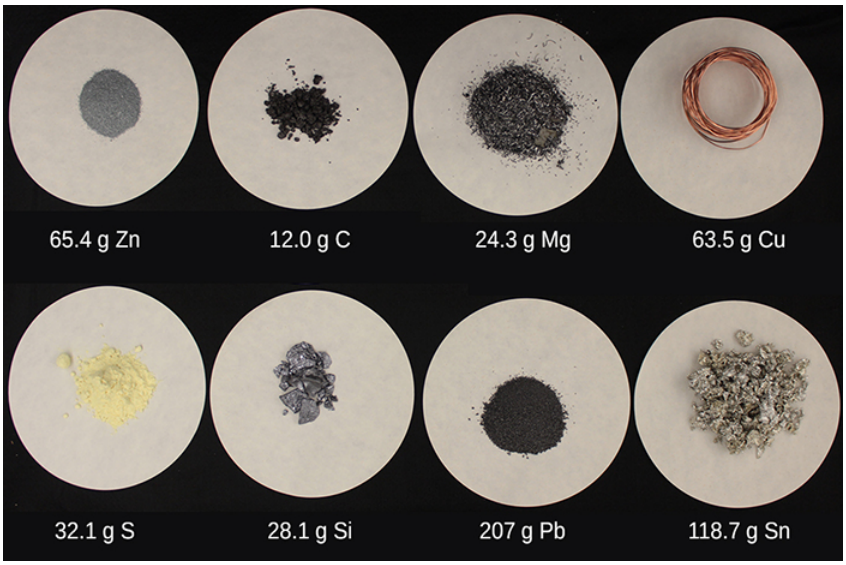


Figure **6.2.4**: Each sample contains 6.022 10^{23} atoms —1.00 mol of atoms. From left to right (top row): 65.4 g zinc, 12.0 g carbon, 24.3 g magnesium, and 63.5 g copper. From left to right (bottom row): 32.1 g sulfur, 28.1 g silicon, 207 g lead, and 118.7 g tin. (credit: modification of work by Mark Ott)

The molar mass of any substance is numerically equivalent to its atomic or formula weight in amu. Per the amu definition, a single ^{12}C atom weighs 12 amu (its atomic mass is 12 amu). A mole of ^{12}C weighs 12 g (its molar mass is 12 g/mol). This relationship holds for all elements, since their atomic masses are measured relative to that of the amu-reference substance, ^{12}C. Extending this principle, the molar mass of a compound in grams is likewise numerically equivalent to its formula mass in amu (Figure **6.2.5**).



Figure **6.2.5**: Each sample contains 6.02 10^{23} molecules or formula units—1.00 mol of the compound or element. Clock-wise from the upper left: 130.2 g of $C_8H_{17}OH$ (1-octanol, formula mass 130.2 amu), 454.4 g of HgI_2 (mercury(II) iodide, formula mass 454.4 amu), 32.0 g of CH_3OH (methanol, formula mass 32.0 amu) and 256.5 g of S_8 (sulfur, formula mass 256.5 amu). (credit: Sahar Atwa)

Element	Average Atomic Mass (amu)	Molar Mass (g/mol)	Atoms/Mole
C	12.01	12.01	6.022 10^{23}
H	1.008	1.008	6.022 10^{23}
O	16.00	16.00	6.022 10^{23}
Na	22.99	22.99	6.022 10^{23}
Cl	35.45	35.45	6.022 10^{23}

While atomic mass and molar mass are numerically equivalent, keep in mind that they are vastly different in terms of scale, as represented by the vast difference in the magnitudes of their respective units (amu versus g). To appreciate the enormity of the mole, consider a small drop of water weighing about 0.03 g (see Figure **6.2.6**). Although this represents just a tiny fraction of 1 mole of water (~18 g), it contains more water molecules than can be clearly imagined. If the molecules were distributed equally among the roughly seven billion people on earth, each person would receive more than 100 billion molecules.



Figure **6.2.6**: The number of molecules in a single droplet of water is roughly 100 billion times greater than the number of people on earth. (credit: "tanakawho"/Wikimedia commons)

Link to Learning

The mole is used in chemistry to represent 6.022 10^{23} of something, but it can be difficult to conceptualize such a large number. Watch this video and then complete the "Think" questions that follow. Explore more about the mole by reviewing the information under "Dig Deeper."

The relationships between formula mass, the mole, and Avogadro's number can be applied to compute various quantities that describe the composition of substances and compounds, as demonstrated in the next several example problems.

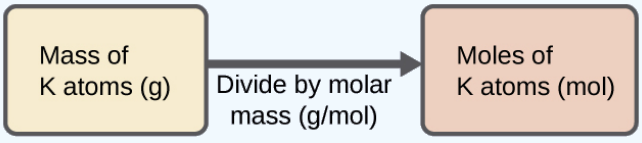
Example 6.2.3: Deriving Moles from Grams for an Element

According to nutritional guidelines from the US Department of Agriculture, the estimated average requirement for dietary potassium is 4.7 g. What is the estimated average requirement of potassium in moles?

Solution

The mass of K is provided, and the corresponding amount of K in moles is requested. Referring to the periodic table, the atomic mass of K is 39.10 amu, and so its molar mass is 39.10 g/mol. The given mass of K (4.7 g) is a bit more than one-tenth the molar mass (39.10 g), so a reasonable "ballpark" estimate of the number of moles would be slightly greater than 0.1 mol.

The molar amount of a substance may be calculated by dividing its mass (g) by its molar mass (g/mol):



The factor-label method supports this mathematical approach since the unit "g" cancels and the answer has units of "mol:"

$$4.7\ \cancel{\text{g K}}\left(\frac{\text{mol K}}{39.10\ \cancel{\text{g K}}}\right) = 0.12\,\text{mol K}$$

The calculated magnitude (0.12 mol K) is consistent with our ballpark expectation, since it is a bit greater than 0.1 mol,

Exercise 6.2.3

Beryllium is a light metal used to fabricate transparent X-ray windows for medical imaging instruments. How many moles of Be are in a thin-foil window weighing 3.24 g?

Answer

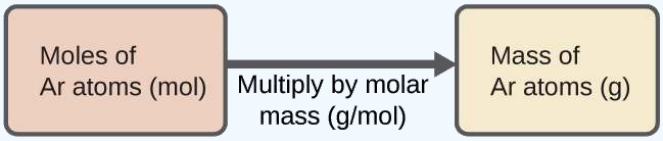
0.360 mol

Example 6.2.4: Deriving Grams from Moles for an Element

A liter of air contains 9.2 10^{-4} mol argon. What is the mass of Ar in a liter of air?

Solution

The molar amount of Ar is provided and must be used to derive the corresponding mass in grams. Since the amount of Ar is less than 1 mole, the mass will be less than the mass of 1 mole of Ar, approximately 40 g. The molar amount in question is approximately one-one thousandth (~10^{-3}) of a mole, and so the corresponding mass should be roughly one-one thousandth of the molar mass (~0.04 g):



In this case, logic dictates (and the factor-label method supports) multiplying the provided amount (mol) by the molar mass (g/mol):

$$9.2 \times 10^{-4} \cancel{\text{mol Ar}} \left(\frac{39.95 \text{ g Ar}}{\cancel{\text{mol Ar}}} \right) = 0.037 \text{ g Ar}$$

The result is in agreement with our expectations, around 0.04 g Ar.

Exercise 6.2.1

What is the mass of 2.561 mol of gold?

Answer

504.4 g

Example 6.2.5: Deriving Number of Atoms from Mass for an Element

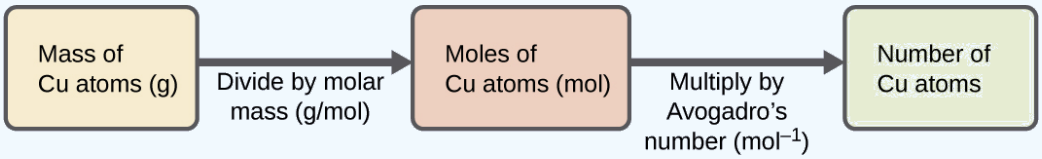
Copper is commonly used to fabricate electrical wire (Figure 6.2.7). How many copper atoms are in 5.00 g of copper wire?



Figure **6.2.7**: Copper wire is composed of many, many atoms of Cu. (credit: Emilian Robert Vicol)

Solution

The number of Cu atoms in the wire may be conveniently derived from its mass by a two-step computation: first calculating the molar amount of Cu, and then using Avogadro's number (N_A) to convert this molar amount to number of Cu atoms:



Considering that the provided sample mass (5.00 g) is a little less than one-tenth the mass of 1 mole of Cu (~64 g), a reasonable estimate for the number of atoms in the sample would be on the order of one-tenth N_A, or approximately 10^{22} Cu atoms. Carrying out the two-step computation yields:

$$5.00\ \cancel{\text{g Cu}} \left(\frac{\cancel{\text{mol Cu}}}{63.55\ \cancel{\text{g Cu}}}\right)\left(\frac{6.022 \times 10^{23}\ \text{Cu atoms}}{\cancel{\text{mol Cu}}}\right) = 4.74 \times 10^{22}\ \text{Cu atoms}$$

The factor-label method yields the desired cancellation of units, and the computed result is on the order of 10^{22} as expected.

? Exercise 6.2.5

A prospector panning for gold in a river collects 15.00 g of pure gold. How many Au atoms are in this quantity of gold?

Answer

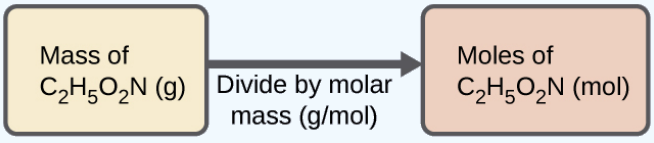
4.586×10^{22} Au atoms

✓ Example 6.2.6: Deriving Moles from Grams for a Compound

Our bodies synthesize protein from amino acids. One of these amino acids is glycine, which has the molecular formula $C_2H_5O_2N$. How many moles of glycine molecules are contained in 28.35 g of glycine?

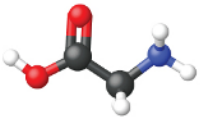
Solution

Derive the number of moles of a compound from its mass following the same procedure used for an element in Example **6.2.3**:



The molar mass of glycine is required for this calculation, and it is computed in the same fashion as its molecular mass. One mole of glycine, $C_2H_5O_2N$, contains 2 moles of carbon, 5 moles of hydrogen, 2 moles of oxygen, and 1 mole of nitrogen:

Element	Quantity (mol element/ mol compound)		Molar mass (g/mol element)		Subtotal (g/mol compound)
C	2	×	12.01	=	24.02
H	5	×	1.008	=	5.040
O	2	×	16.00	=	32.00
N	1	×	14.007	=	14.007
Molecular mass (g/mol compound)					75.07



The provided mass of glycine (~28 g) is a bit more than one-third the molar mass (~75 g/mol), so the computed result is expected to be a bit greater than one-third of a mole (~0.33 mol). Dividing the compound's mass by its molar mass yields:

$$28.35 \cancel{\text{ g glycine}} \left(\frac{\text{mol glycine}}{75.07 \cancel{\text{ g glycine}}} \right) = 0.378 \text{ mol glycine}$$

This result is consistent with the rough estimate,

? Exercise 6.2.6

How many moles of sucrose, $C_{12}H_{22}O_{11}$, are in a 25-g sample of sucrose?

Answer

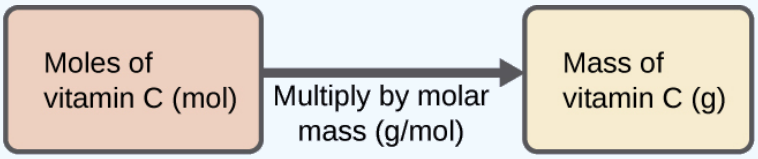
0.073 mol

✓ Example 6.2.7: Deriving Grams from Moles for a Compound

Vitamin C is a covalent compound with the molecular formula $C_6H_8O_6$. The recommended daily dietary allowance of vitamin C for children aged 4–8 years is $1.42\ 10^{-4}$ mol. What is the mass of this allowance in grams?

Solution

As for elements, the mass of a compound can be derived from its molar amount as shown:



The molar mass for this compound is computed to be 176.124 g/mol. The given number of moles is a very small fraction of a mole (~10^{-4} or one-ten thousandth); therefore, the corresponding mass is expected to be about one-ten thousandth of the molar mass (~0.02 g). Performing the calculation yields:

$$1.42 \times 10^{-4} \cancel{\text{ mol vitamin C}} \left(\frac{176.124 \text{ g vitamin C}}{\cancel{\text{mol vitamin C}}} \right) = 0.0250 \text{ g vitamin C}$$

This is consistent with the anticipated result.

? Exercise 6.2.7

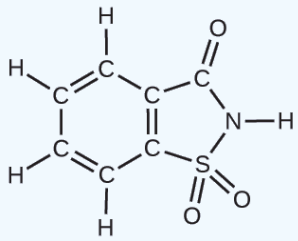
What is the mass of 0.443 mol of hydrazine, N_2H_4?

Answer

14.2 g

Example 6.2.8: Deriving the Number of Atoms and Molecules from the Mass of a Compound

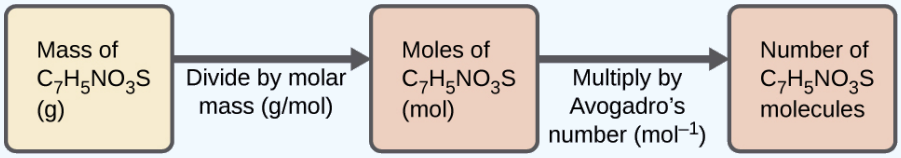
A packet of an artificial sweetener contains 40.0 mg of saccharin ($C_7H_5NO_3S$), which has the structural formula:



Given that saccharin has a molar mass of 183.18 g/mol, how many saccharin molecules are in a 40.0-mg (0.0400-g) sample of saccharin? How many carbon atoms are in the same sample?

Solution

The number of molecules in a given mass of compound is computed by first deriving the number of moles, as demonstrated in Example **6.2.6**, and then multiplying by Avogadro's number:



Using the provided mass and molar mass for saccharin yields:

$$0.0400\ \cancel{\text{g } C_7H_5NO_3S}\left(\frac{\cancel{\text{mol } C_7H_5NO_3S}}{183.18\ \cancel{\text{g } CH_5NO_3S}}\right)\left(\frac{6.022\times10^{23}\ C_7H_5NO_3S\text{ molecules}}{1\ \cancel{\text{mol } C_7H_5NO_3S}}\right)$$
$$= 1.31\times10^{20}\ C_7H_5NO_3S\text{ molecules}$$

The compound's formula shows that each molecule contains seven carbon atoms, and so the number of C atoms in the provided sample is:

$$1.31\times10^{20}\ C_7H_5NO_3S\text{ molecules}\left(\frac{7\ C\text{ atoms}}{1\ C_7H_5NO_3S\text{ molecule}}\right) = 9.17\times10^{20}\ C\text{ atoms}$$

Exercise 6.2.8

How many C_4H_{10} molecules are contained in 9.213 g of this compound? How many hydrogen atoms?

Answer

9.545×10^{22} molecules C_4H_{10}

9.545×10^{23} atoms H

How Sciences Interconnect: Counting Neurotransmitter Molecules in the Brain

The brain is the control center of the central nervous system (Figure **6.2.8**). It sends and receives signals to and from muscles and other internal organs to monitor and control their functions; it processes stimuli detected by sensory organs to guide interactions with the external world; and it houses the complex physiological processes that give rise to our intellect and emotions. The broad field of neuroscience spans all aspects of the structure and function of the central nervous system, including research on the anatomy and physiology of the brain. Great progress has been made in brain research over the past few decades, and the BRAIN Initiative, a federal initiative announced in 2013, aims to accelerate and capitalize on these

advances through the concerted efforts of various industrial, academic, and government agencies (more details available at www.whitehouse.gov/share/brain-initiative).

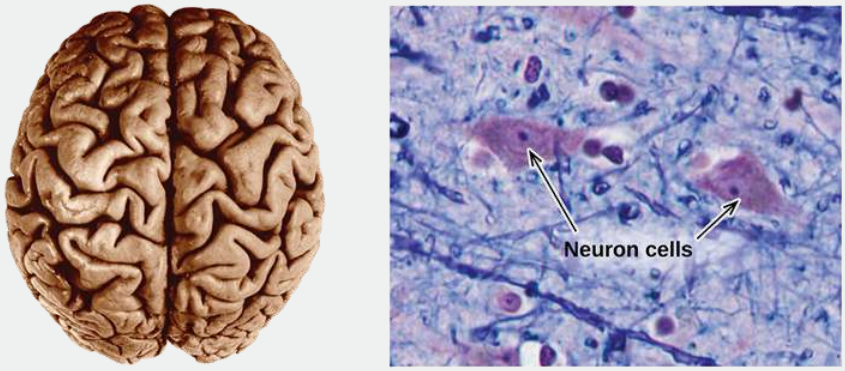


Figure **6.2.8**: (a) A typical human brain weighs about 1.5 kg and occupies a volume of roughly 1.1 L. (b) Information is transmitted in brain tissue and throughout the central nervous system by specialized cells called neurons (micrograph shows cells at 1600× magnification).

Specialized cells called neurons transmit information between different parts of the central nervous system by way of electrical and chemical signals. Chemical signaling occurs at the interface between different neurons when one of the cells releases molecules (called neurotransmitters) that diffuse across the small gap between the cells (called the synapse) and bind to the surface of the other cell. These neurotransmitter molecules are stored in small intracellular structures called vesicles that fuse to the cell membrane and then break open to release their contents when the neuron is appropriately stimulated. This process is called exocytosis (see Figure **6.2.9**). One neurotransmitter that has been very extensively studied is dopamine, $C_8H_{11}NO_2$. Dopamine is involved in various neurological processes that impact a wide variety of human behaviors. Dysfunctions in the dopamine systems of the brain underlie serious neurological diseases such as Parkinson's and schizophrenia.

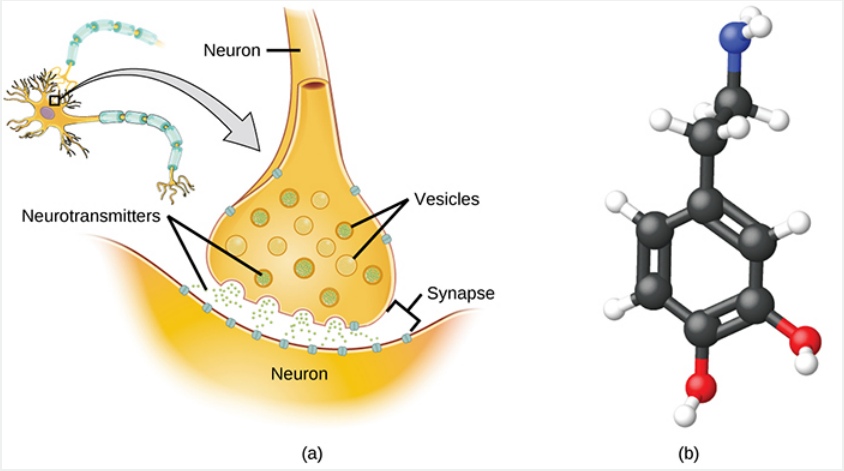


Figure **6.2.9**: (a) Chemical signals are transmitted from neurons to other cells by the release of neurotransmitter molecules into the small gaps (synapses) between the cells. (b) Dopamine, $C_8H_{11}NO_2$, is a neurotransmitter involved in a number of neurological processes.

One important aspect of the complex processes related to dopamine signaling is the number of neurotransmitter molecules released during exocytosis. Since this number is a central factor in determining neurological response (and subsequent human thought and action), it is important to know how this number changes with certain controlled stimulations, such as the administration of drugs. It is also important to understand the mechanism responsible for any changes in the number of neurotransmitter molecules released—for example, some dysfunction in exocytosis, a change in the number of vesicles in the neuron, or a change in the number of neurotransmitter molecules in each vesicle.

Significant progress has been made recently in directly measuring the number of dopamine molecules stored in individual vesicles and the amount actually released when the vesicle undergoes exocytosis. Using miniaturized probes that can

selectively detect dopamine molecules in very small amounts, scientists have determined that the vesicles of a certain type of mouse brain neuron contain an average of 30,000 dopamine molecules per vesicle (about 5×10^{-20} mol or 50 zmol). Analysis of these neurons from mice subjected to various drug therapies shows significant changes in the average number of dopamine molecules contained in individual vesicles, increasing or decreasing by up to three-fold, depending on the specific drug used. These studies also indicate that not all of the dopamine in a given vesicle is released during exocytosis, suggesting that it may be possible to regulate the fraction released using pharmaceutical therapies.

6.2.3: Footnotes

- 1Omiatek, Donna M., Amanda J. Bressler, Ann-Sofie Cans, Anne M. Andrews, Michael L. Heien, and Andrew G. Ewing. "The Real Catecholamine Content of Secretory Vesicles in the CNS Revealed by Electrochemical Cytometry." *Scientific Report* 3 (2013): 1447, accessed January 14, 2015, doi:10.1038/srep01447.

This page titled 6.2: Formula Mass is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **3.1: Formula Mass and the Mole Concept** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

6.3: Converting between Grams and Moles

Learning Objectives

By the end of this section, you will be able to:

- Calculate formula masses for covalent and ionic compounds
- Define the amount unit mole and the related quantity Avogadro's number Explain the relation between mass, moles, and numbers of atoms or molecules, and perform calculations deriving these quantities from one another

Many argue that modern chemical science began when scientists started exploring the quantitative as well as the qualitative aspects of chemistry. For example, Dalton's atomic theory was an attempt to explain the results of measurements that allowed him to calculate the relative masses of elements combined in various compounds. Understanding the relationship between the masses of atoms and the chemical formulas of compounds allows us to quantitatively describe the composition of substances.

6.3.1: Formula Mass

An earlier chapter of this text described the development of the atomic mass unit, the concept of average atomic masses, and the use of chemical formulas to represent the elemental makeup of substances. These ideas can be extended to calculate the formula mass of a substance by summing the average atomic masses of all the atoms represented in the substance's formula.

6.3.1.1: Formula Mass for Covalent Substances

For covalent substances, the formula represents the numbers and types of atoms composing a single molecule of the substance; therefore, the formula mass may be correctly referred to as a molecular mass. Consider chloroform ($\mathbf{CHCl_3}$), a covalent compound once used as a surgical anesthetic and now primarily used in the production of tetrafluoroethylene, the building block for the "anti-stick" polymer, Teflon. The molecular formula of chloroform indicates that a single molecule contains one carbon atom, one hydrogen atom, and three chlorine atoms. The average molecular mass of a chloroform molecule is therefore equal to the sum of the average atomic masses of these atoms. Figure **6.3.1** outlines the calculations used to derive the molecular mass of chloroform, which is 119.37 amu.

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	1	×	12.01	=	12.01
H	1	×	1.008	=	1.008
Cl	3	×	35.45	=	106.35
				Molecular mass	119.37

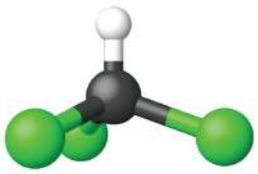


Figure **6.3.1**: The average mass of a chloroform molecule, $CHCl_3$, is 119.37 amu, which is the sum of the average atomic masses of each of its constituent atoms. The model shows the molecular structure of chloroform.

Likewise, the molecular mass of an aspirin molecule, $\mathbf{C_9H_8O_4}$, is the sum of the atomic masses of nine carbon atoms, eight hydrogen atoms, and four oxygen atoms, which amounts to 180.15 amu (Figure **6.3.2**).

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	9	×	12.01	=	108.09
H	8	×	1.008	=	8.064
O	4	×	16.00	=	64.00
				Molecular mass	180.15

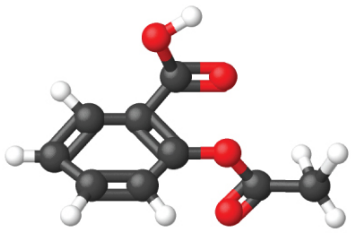


Figure **6.3.2**: The average mass of an aspirin molecule is 180.15 amu. The model shows the molecular structure of aspirin, $C_9H_8O_4$.

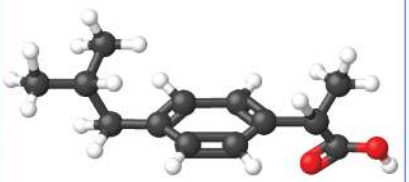
Example 6.3.1: Computing Molecular Mass for a Covalent Compound

Ibuprofen, $C_{13}H_{18}O_2$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Advil and Motrin. What is the molecular mass (amu) for this compound?

Solution

Molecules of this compound are composed of 13 carbon atoms, 18 hydrogen atoms, and 2 oxygen atoms. Following the approach described above, the average molecular mass for this compound is therefore:

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
C	13	×	12.01	=	156.13
H	18	×	1.008	=	18.144
O	2	×	16.00	=	32.00
				Molecular mass	206.27



Exercise 6.3.1

Acetaminophen, $C_8H_9NO_2$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Tylenol. What is the molecular mass (amu) for this compound?

Answer

151.16 amu

6.3.1.2: Formula Mass for Ionic Compounds

Ionic compounds are composed of discrete cations and anions combined in ratios to yield electrically neutral bulk matter. The formula mass for an ionic compound is calculated in the same way as the formula mass for covalent compounds: by summing the average atomic masses of all the atoms in the compound's formula. Keep in mind, however, that the formula for an ionic compound does not represent the composition of a discrete molecule, so it may not correctly be referred to as the "molecular mass."

As an example, consider sodium chloride, NaCl, the chemical name for common table salt. Sodium chloride is an ionic compound composed of sodium cations, Na^+, and chloride anions, Cl^-, combined in a 1:1 ratio. The formula mass for this compound is computed as 58.44 amu (see Figure **6.3.3**).

Element	Quantity		Average atomic mass (amu)		Subtotal
Na	1	×	22.99	=	22.99
Cl	1	×	35.45	=	35.45
				Formula mass	58.44

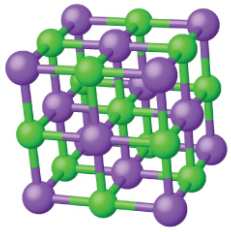


Figure **6.3.3**: Table salt, NaCl, contains an array of sodium and chloride ions combined in a 1:1 ratio. Its formula mass is 58.44 amu.

Note that the average masses of neutral sodium and chlorine atoms were used in this computation, rather than the masses for sodium cations and chlorine anions. This approach is perfectly acceptable when computing the formula mass of an ionic compound. Even though a sodium cation has a slightly smaller mass than a sodium atom (since it is missing an electron), this difference will be offset by the fact that a chloride anion is slightly more massive than a chloride atom (due to the extra electron). Moreover, the mass of an electron is negligibly small with respect to the mass of a typical atom. Even when calculating the mass of an isolated ion, the missing or additional electrons can generally be ignored, since their contribution to the overall mass is negligible, reflected only in the nonsignificant digits that will be lost when the computed mass is properly rounded. The few exceptions to this guideline are very light ions derived from elements with precisely known atomic masses.

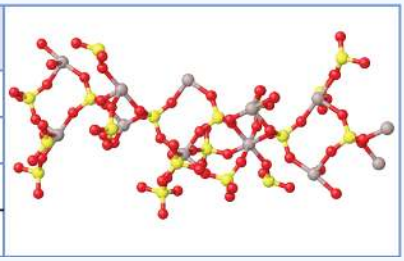
Example 6.3.2: Computing Formula Mass for an Ionic Compound

Aluminum sulfate, $Al_2(SO_4)_3$, is an ionic compound that is used in the manufacture of paper and in various water purification processes. What is the formula mass (amu) of this compound?

Solution

The formula for this compound indicates it contains Al^{3+} and SO_4^{2-} ions combined in a 2:3 ratio. For purposes of computing a formula mass, it is helpful to rewrite the formula in the simpler format, $Al_2S_3O_{12}$. Following the approach outlined above, the formula mass for this compound is calculated as follows:

Element	Quantity		Average atomic mass (amu)		Subtotal (amu)
Al	2	×	26.98	=	53.96
S	3	×	32.06	=	96.18
O	12	×	16.00	=	192.00
				Molecular mass	342.14



Exercise 6.3.2

Calcium phosphate, $Ca_3(PO_4)_2$, is an ionic compound and a common anti-caking agent added to food products. What is the formula mass (amu) of calcium phosphate?

Answer

310.18 amu

6.3.2: The Mole

The identity of a substance is defined not only by the types of atoms or ions it contains, but by the quantity of each type of atom or ion. For example, water, H_2O, and hydrogen peroxide, H_2O_2, are alike in that their respective molecules are composed of hydrogen and oxygen atoms. However, because a hydrogen peroxide molecule contains two oxygen atoms, as opposed to the water molecule, which has only one, the two substances exhibit very different properties. Today, sophisticated instruments allow the direct measurement of these defining microscopic traits; however, the same traits were originally derived from the measurement of macroscopic properties (the masses and volumes of bulk quantities of matter) using relatively simple tools (balances and volumetric glassware). This experimental approach required the introduction of a new unit for amount of substances, the *mole*, which remains indispensable in modern chemical science.

The *mole* is an amount unit similar to familiar units like pair, dozen, gross, etc. It provides a specific measure of *the number* of atoms or molecules in a sample of matter. One Latin connotation for the word “mole” is “large mass” or “bulk,” which is consistent with its use as the name for this unit. The mole provides a link between an easily measured macroscopic property, bulk mass, and an extremely important fundamental property, number of atoms, molecules, and so forth. A mole of substance is that amount in which there are $6.02214076 \times 10^{23}$.

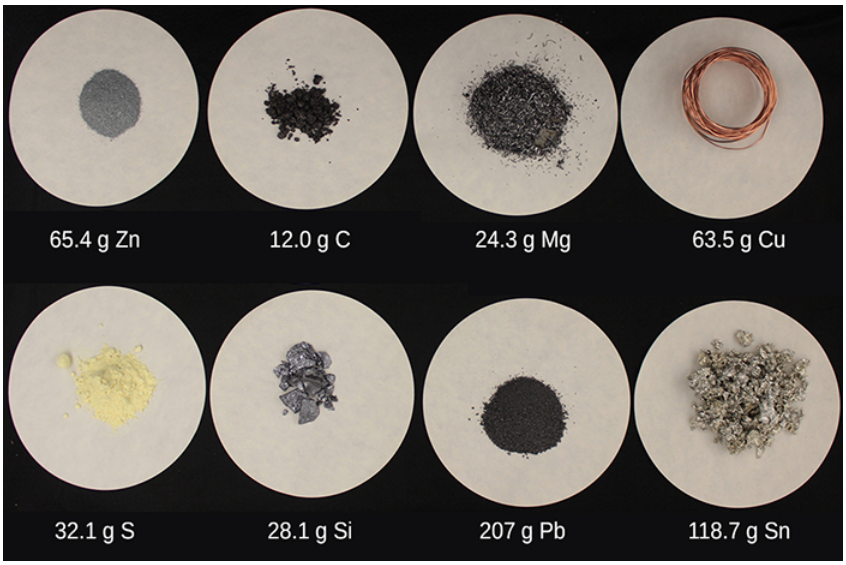


Figure **6.3.4**: Each sample contains 6.022 10^{23} atoms —1.00 mol of atoms. From left to right (top row): 65.4 g zinc, 12.0 g carbon, 24.3 g magnesium, and 63.5 g copper. From left to right (bottom row): 32.1 g sulfur, 28.1 g silicon, 207 g lead, and 118.7 g tin. (credit: modification of work by Mark Ott)

The molar mass of any substance is numerically equivalent to its atomic or formula weight in amu. Per the amu definition, a single ^{12}C atom weighs 12 amu (its atomic mass is 12 amu). A mole of ^{12}C weighs 12 g (its molar mass is 12 g/mol). This relationship holds for all elements, since their atomic masses are measured relative to that of the amu-reference substance, ^{12}C. Extending this principle, the molar mass of a compound in grams is likewise numerically equivalent to its formula mass in amu (Figure **6.3.5**).



Figure **6.3.5**: Each sample contains 6.02 10^{23} molecules or formula units—1.00 mol of the compound or element. Clock-wise from the upper left: 130.2 g of $C_8H_{17}OH$ (1-octanol, formula mass 130.2 amu), 454.4 g of HgI_2 (mercury(II) iodide, formula mass 454.4 amu), 32.0 g of CH_3OH (methanol, formula mass 32.0 amu) and 256.5 g of S_8 (sulfur, formula mass 256.5 amu). (credit: Sahar Atwa)

Element	Average Atomic Mass (amu)	Molar Mass (g/mol)	Atoms/Mole
C	12.01	12.01	6.022 10^{23}
H	1.008	1.008	6.022 10^{23}
O	16.00	16.00	6.022 10^{23}
Na	22.99	22.99	6.022 10^{23}
Cl	35.45	35.45	6.022 10^{23}

While atomic mass and molar mass are numerically equivalent, keep in mind that they are vastly different in terms of scale, as represented by the vast difference in the magnitudes of their respective units (amu versus g). To appreciate the enormity of the mole, consider a small drop of water weighing about 0.03 g (see Figure **6.3.6**). Although this represents just a tiny fraction of 1 mole of water (~18 g), it contains more water molecules than can be clearly imagined. If the molecules were distributed equally among the roughly seven billion people on earth, each person would receive more than 100 billion molecules.



Figure **6.3.6**: The number of molecules in a single droplet of water is roughly 100 billion times greater than the number of people on earth. (credit: "tanakawho"/Wikimedia commons)

Link to Learning

The mole is used in chemistry to represent 6.022 10^{23} of something, but it can be difficult to conceptualize such a large number. Watch this video and then complete the "Think" questions that follow. Explore more about the mole by reviewing the information under "Dig Deeper."

The relationships between formula mass, the mole, and Avogadro's number can be applied to compute various quantities that describe the composition of substances and compounds, as demonstrated in the next several example problems.

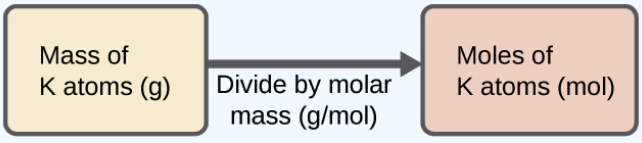
Example 6.3.3: Deriving Moles from Grams for an Element

According to nutritional guidelines from the US Department of Agriculture, the estimated average requirement for dietary potassium is 4.7 g. What is the estimated average requirement of potassium in moles?

Solution

The mass of K is provided, and the corresponding amount of K in moles is requested. Referring to the periodic table, the atomic mass of K is 39.10 amu, and so its molar mass is 39.10 g/mol. The given mass of K (4.7 g) is a bit more than one-tenth the molar mass (39.10 g), so a reasonable "ballpark" estimate of the number of moles would be slightly greater than 0.1 mol.

The molar amount of a substance may be calculated by dividing its mass (g) by its molar mass (g/mol):



The factor-label method supports this mathematical approach since the unit "g" cancels and the answer has units of "mol:"

$$4.7\ \cancel{\text{g K}}\left(\frac{\text{mol K}}{39.10\ \cancel{\text{g K}}}\right) = 0.12\,\text{mol K}$$

The calculated magnitude (0.12 mol K) is consistent with our ballpark expectation, since it is a bit greater than 0.1 mol,

Exercise 6.3.3

Beryllium is a light metal used to fabricate transparent X-ray windows for medical imaging instruments. How many moles of Be are in a thin-foil window weighing 3.24 g?

Answer

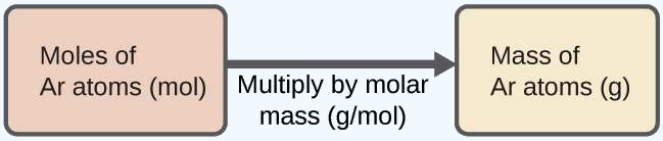
0.360 mol

Example 6.3.4: Deriving Grams from Moles for an Element

A liter of air contains 9.2 10^{-4} mol argon. What is the mass of Ar in a liter of air?

Solution

The molar amount of Ar is provided and must be used to derive the corresponding mass in grams. Since the amount of Ar is less than 1 mole, the mass will be less than the mass of 1 mole of Ar, approximately 40 g. The molar amount in question is approximately one-one thousandth (~10^{-3}) of a mole, and so the corresponding mass should be roughly one-one thousandth of the molar mass (~0.04 g):



In this case, logic dictates (and the factor-label method supports) multiplying the provided amount (mol) by the molar mass (g/mol):

$$9.2 \times 10^{-4} \cancel{\text{mol Ar}} \left(\frac{39.95 \text{ g Ar}}{\cancel{\text{mol Ar}}} \right) = 0.037 \text{ g Ar}$$

The result is in agreement with our expectations, around 0.04 g Ar.

Exercise 6.3.1

What is the mass of 2.561 mol of gold?

Answer

504.4 g

Example 6.3.5: Deriving Number of Atoms from Mass for an Element

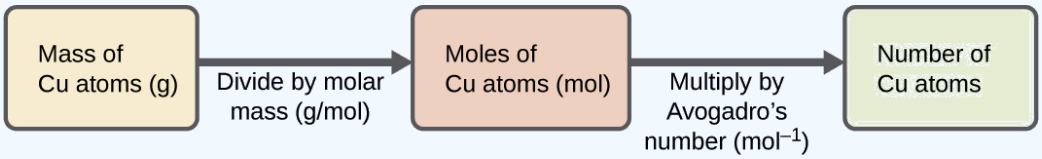
Copper is commonly used to fabricate electrical wire (Figure 6.3.7). How many copper atoms are in 5.00 g of copper wire?



Figure **6.3.7**: Copper wire is composed of many, many atoms of Cu. (credit: Emilian Robert Vicol)

Solution

The number of Cu atoms in the wire may be conveniently derived from its mass by a two-step computation: first calculating the molar amount of Cu, and then using Avogadro's number (N_A) to convert this molar amount to number of Cu atoms:



Considering that the provided sample mass (5.00 g) is a little less than one-tenth the mass of 1 mole of Cu (~64 g), a reasonable estimate for the number of atoms in the sample would be on the order of one-tenth N_A, or approximately 10^{22} Cu atoms. Carrying out the two-step computation yields:

$$5.00\ \cancel{\text{g Cu}} \left(\frac{\cancel{\text{mol Cu}}}{63.55\ \cancel{\text{g Cu}}}\right)\left(\frac{6.022 \times 10^{23}\ \text{Cu atoms}}{\cancel{\text{mol Cu}}}\right) = 4.74 \times 10^{22}\ \text{Cu atoms}$$

The factor-label method yields the desired cancellation of units, and the computed result is on the order of 10^{22} as expected.

? Exercise 6.3.5

A prospector panning for gold in a river collects 15.00 g of pure gold. How many Au atoms are in this quantity of gold?

Answer

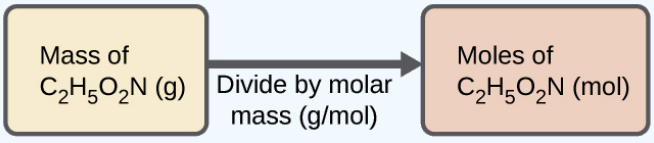
4.586×10^{22} Au atoms

✓ Example 6.3.6: Deriving Moles from Grams for a Compound

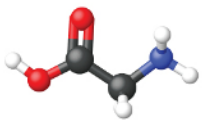
Our bodies synthesize protein from amino acids. One of these amino acids is glycine, which has the molecular formula $C_2H_5O_2N$. How many moles of glycine molecules are contained in 28.35 g of glycine?

Solution

Derive the number of moles of a compound from its mass following the same procedure used for an element in Example **6.3.3**:



The molar mass of glycine is required for this calculation, and it is computed in the same fashion as its molecular mass. One mole of glycine, $C_2H_5O_2N$, contains 2 moles of carbon, 5 moles of hydrogen, 2 moles of oxygen, and 1 mole of nitrogen:

Element	Quantity (mol element/ mol compound)		Molar mass (g/mol element)		Subtotal (g/mol compound)	
C	2	×	12.01	=	24.02	
H	5	×	1.008	=	5.040	
O	2	×	16.00	=	32.00	
N	1	×	14.007	=	14.007	
Molecular mass (g/mol compound)					75.07	

The provided mass of glycine (~28 g) is a bit more than one-third the molar mass (~75 g/mol), so the computed result is expected to be a bit greater than one-third of a mole (~0.33 mol). Dividing the compound's mass by its molar mass yields:

$$28.35 \cancel{\text{ g glycine}} \left(\frac{\text{mol glycine}}{75.07 \cancel{\text{ g glycine}}} \right) = 0.378 \text{ mol glycine}$$

This result is consistent with the rough estimate,

? Exercise 6.3.6

How many moles of sucrose, $C_{12}H_{22}O_{11}$, are in a 25-g sample of sucrose?

Answer

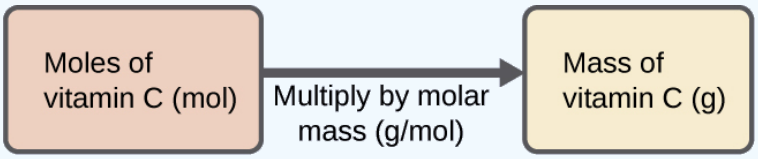
0.073 mol

✓ Example 6.3.7: Deriving Grams from Moles for a Compound

Vitamin C is a covalent compound with the molecular formula $C_6H_8O_6$. The recommended daily dietary allowance of vitamin C for children aged 4–8 years is $1.42\ 10^{-4}$ mol. What is the mass of this allowance in grams?

Solution

As for elements, the mass of a compound can be derived from its molar amount as shown:



The molar mass for this compound is computed to be 176.124 g/mol. The given number of moles is a very small fraction of a mole (~10^{-4} or one-ten thousandth); therefore, the corresponding mass is expected to be about one-ten thousandth of the molar mass (~0.02 g). Performing the calculation yields:

$$1.42 \times 10^{-4} \cancel{\text{ mol vitamin C}} \left(\frac{176.124 \text{ g vitamin C}}{\cancel{\text{mol vitamin C}}} \right) = 0.0250 \text{ g vitamin C}$$

This is consistent with the anticipated result.

? Exercise 6.3.7

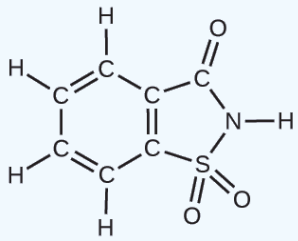
What is the mass of 0.443 mol of hydrazine, N_2H_4?

Answer

14.2 g

Example 6.3.8: Deriving the Number of Atoms and Molecules from the Mass of a Compound

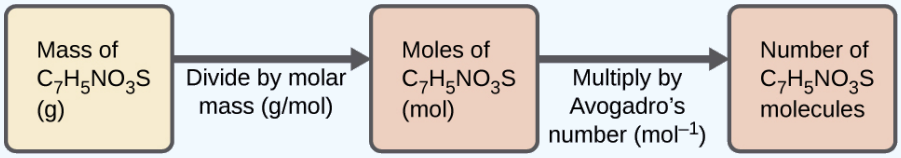
A packet of an artificial sweetener contains 40.0 mg of saccharin ($C_7H_5NO_3S$), which has the structural formula:



Given that saccharin has a molar mass of 183.18 g/mol, how many saccharin molecules are in a 40.0-mg (0.0400-g) sample of saccharin? How many carbon atoms are in the same sample?

Solution

The number of molecules in a given mass of compound is computed by first deriving the number of moles, as demonstrated in Example **6.3.6**, and then multiplying by Avogadro's number:



Using the provided mass and molar mass for saccharin yields:

$$0.0400\ \cancel{\text{g } C_7H_5NO_3S}\left(\frac{\cancel{\text{mol } C_7H_5NO_3S}}{183.18\ \cancel{\text{g } CH_5NO_3S}}\right)\left(\frac{6.022\times10^{23}\ C_7H_5NO_3S\text{ molecules}}{1\ \cancel{\text{mol } C_7H_5NO_3S}}\right)$$
$$= 1.31\times10^{20}\ C_7H_5NO_3S\text{ molecules}$$

The compound's formula shows that each molecule contains seven carbon atoms, and so the number of C atoms in the provided sample is:

$$1.31\times10^{20}\ C_7H_5NO_3S\text{ molecules}\left(\frac{7\ C\text{ atoms}}{1\ C_7H_5NO_3S\text{ molecule}}\right) = 9.17\times10^{20}\ C\text{ atoms}$$

Exercise 6.3.8

How many C_4H_{10} molecules are contained in 9.213 g of this compound? How many hydrogen atoms?

Answer

9.545×10^{22} molecules C_4H_{10}

9.545×10^{23} atoms H

How Sciences Interconnect: Counting Neurotransmitter Molecules in the Brain

The brain is the control center of the central nervous system (Figure **6.3.8**). It sends and receives signals to and from muscles and other internal organs to monitor and control their functions; it processes stimuli detected by sensory organs to guide interactions with the external world; and it houses the complex physiological processes that give rise to our intellect and emotions. The broad field of neuroscience spans all aspects of the structure and function of the central nervous system, including research on the anatomy and physiology of the brain. Great progress has been made in brain research over the past few decades, and the BRAIN Initiative, a federal initiative announced in 2013, aims to accelerate and capitalize on these

advances through the concerted efforts of various industrial, academic, and government agencies (more details available at www.whitehouse.gov/share/brain-initiative).

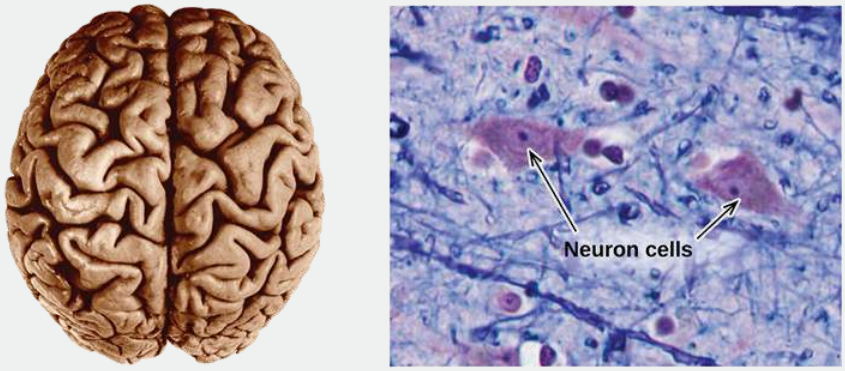


Figure **6.3.8**: (a) A typical human brain weighs about 1.5 kg and occupies a volume of roughly 1.1 L. (b) Information is transmitted in brain tissue and throughout the central nervous system by specialized cells called neurons (micrograph shows cells at 1600× magnification).

Specialized cells called neurons transmit information between different parts of the central nervous system by way of electrical and chemical signals. Chemical signaling occurs at the interface between different neurons when one of the cells releases molecules (called neurotransmitters) that diffuse across the small gap between the cells (called the synapse) and bind to the surface of the other cell. These neurotransmitter molecules are stored in small intracellular structures called vesicles that fuse to the cell membrane and then break open to release their contents when the neuron is appropriately stimulated. This process is called exocytosis (see Figure **6.3.9**). One neurotransmitter that has been very extensively studied is dopamine, $C_8H_{11}NO_2$. Dopamine is involved in various neurological processes that impact a wide variety of human behaviors. Dysfunctions in the dopamine systems of the brain underlie serious neurological diseases such as Parkinson's and schizophrenia.

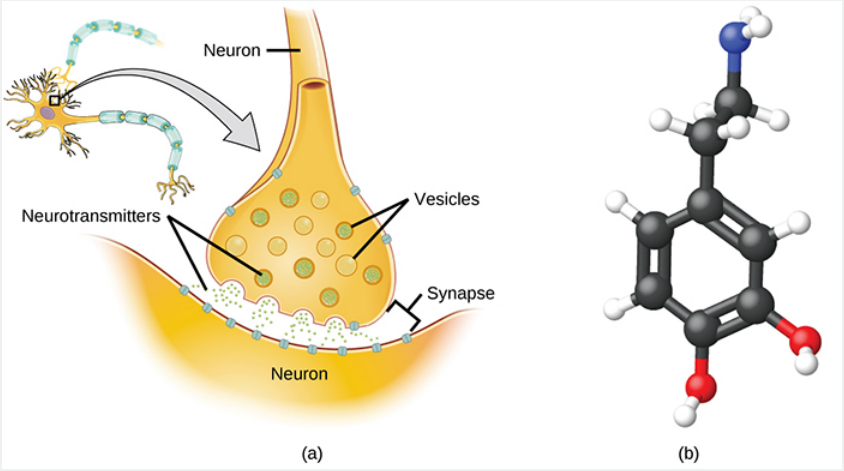


Figure **6.3.9**: (a) Chemical signals are transmitted from neurons to other cells by the release of neurotransmitter molecules into the small gaps (synapses) between the cells. (b) Dopamine, $C_8H_{11}NO_2$, is a neurotransmitter involved in a number of neurological processes.

One important aspect of the complex processes related to dopamine signaling is the number of neurotransmitter molecules released during exocytosis. Since this number is a central factor in determining neurological response (and subsequent human thought and action), it is important to know how this number changes with certain controlled stimulations, such as the administration of drugs. It is also important to understand the mechanism responsible for any changes in the number of neurotransmitter molecules released—for example, some dysfunction in exocytosis, a change in the number of vesicles in the neuron, or a change in the number of neurotransmitter molecules in each vesicle.

Significant progress has been made recently in directly measuring the number of dopamine molecules stored in individual vesicles and the amount actually released when the vesicle undergoes exocytosis. Using miniaturized probes that can

selectively detect dopamine molecules in very small amounts, scientists have determined that the vesicles of a certain type of mouse brain neuron contain an average of 30,000 dopamine molecules per vesicle (about 5×10^{-20} mol or 50 zmol). Analysis of these neurons from mice subjected to various drug therapies shows significant changes in the average number of dopamine molecules contained in individual vesicles, increasing or decreasing by up to three-fold, depending on the specific drug used. These studies also indicate that not all of the dopamine in a given vesicle is released during exocytosis, suggesting that it may be possible to regulate the fraction released using pharmaceutical therapies.

6.3.3: Footnotes

- 1Omiatek, Donna M., Amanda J. Bressler, Ann-Sofie Cans, Anne M. Andrews, Michael L. Heien, and Andrew G. Ewing. "The Real Catecholamine Content of Secretory Vesicles in the CNS Revealed by Electrochemical Cytometry." *Scientific Report* 3 (2013): 1447, accessed January 14, 2015, doi:10.1038/srep01447.

This page titled 6.3: Converting between Grams and Moles is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **3.1: Formula Mass and the Mole Concept** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

6.4: Case Study- The Mole Concept in Clinical Laboratory Analysis

Introduction: The mole is a fundamental unit in chemistry that quantifies the amount of a substance. In a clinical laboratory setting, the concept of moles is pivotal for determining the concentrations of various substances in patient samples. This case study examines how laboratory technicians apply the mole concept to analyze glucose concentration in blood samples, a routine yet critical procedure in diagnosing and monitoring conditions such as diabetes.

Scenario: In City Hospital's clinical laboratory, a team of skilled technicians, including John, is working to determine the glucose levels in blood samples from a diverse patient pool. They are using a colorimetric assay that quantifies glucose concentration based on the color intensity of the reaction product. For accurate diagnosis and treatment monitoring, John must calculate the molarity of glucose—moles of glucose per liter of solution. This requires him to understand and apply the mole concept accurately.

Application of Moles in Clinical Analysis: John knows that one mole of any substance contains Avogadro's number of entities (atoms, ions, molecules), which is 6.022×10236.022×1023. He uses this information in clinical assays to convert between moles and concentrations. By measuring how much light is absorbed by the sample, he can infer the number of moles of glucose in the blood and thus its concentration.

Case Study Questions:

1. **How is the concept of moles applied in clinical laboratory analysis?**
2. **Explain how moles are related to formula mass.**

Hands-On Classroom Activities:

1. **Moles in Medicine:** In the educational task "Moles in Medicine," students are assigned to calculate the number of moles present in samples of common medications. They will then be asked to correlate their findings with clinical dosing guidelines, thus reinforcing the practical application of mole concepts in a real-world medical context.

Conclusion: In the clinical laboratory, the mole concept is not just an abstract principle but a daily tool that technicians like John rely on to provide accurate and life-critical information. The precision of their measurements and calculations can directly influence patient care outcomes. Understanding the mole concept and its relation to formula mass enables technicians to convert mass measurements into meaningful molar concentrations, which are essential for diagnosing and managing medical conditions.

6.4: Case Study- The Mole Concept in Clinical Laboratory Analysis is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

6.E: Exercises

Multiple Choice Questions

1. What quantity gives the number of atoms in a mole?
   a. Avogadro's number
   b. Formula mass
   c. Molar mass
   d. Gas constant
2. What is the formula mass of $MgCl_2$?
   a. 59.76 amu
   b. 95.21 amu
   c. 119.5 amu
   d. 125.8 amu
3. What is the formula mass of potassium sulfide?
   a. 39.10 amu
   b. 71.16 amu
   c. 103.2 amu
   d. 110.3 amu
4. A 1.00-carat diamond has a mass of 0.200 g. Which of the following gives the correct number of carbon atoms in a 1.00-carat diamond?
   a. 3.99×10^{-24} carbon atoms
   b. 1.00×10^{23} carbon atoms
   c. 1.20×10^{23} carbon atoms
   d. 1.45×10^{24} carbon atoms
5. How many moles of oxygen are present in 3 moles of sodium sulfate?
   a. 3
   b. 4
   c. 9
   d. 12
6. How many moles of CCl_4 are present in a 7.82 g sample of this substance?
   a. 0.0102 mol
   b. 0.0508 mol
   c. 0.106 mol
   d. 0.254 mol
7. Which of the following gives the correct mass (in amu) of F in the compound boron trifluoride?
   a. 19.00 amu
   b. 38.00 amu

c. 57.00 amu

d. 114.0 amu

8. What mass of Fe contains 2.60×10^{24} atoms of Fe?

a. 241 g

b. 77.3 mg

c. 2.41 kg

d. 4.32×10^{46} g

9. A saline solution used for an intravenous drip contains 9.0 g of sodium chloride per liter of solution. How many sodium ions are present in a 150 mL quantity of saline solution?

a. 1.7×10^{20}

b. 1.4×10^{22}

c. 3.4×10^{23}

d. 5.9×10^{23}

10. The chemical formula for the medication IMBRUVICA® is $C_{25}H_{24}N_6O_2$. How many atoms of C are present in a 422 mg sample of this medication?

a. 5.77×10^{20}

b. 1.44×10^{22}

c. 3.29×10^{22}

d. 2.80×10^{27}

Easy

1. How many peas are in 2.0 moles of peas?

2. There are approximately 7×10^{23} stars in the universe. How many moles of stars does this correspond to? In comparison, there are approximately 7.5×10^{18} grains of sand on the earth. How many moles does this correspond to?

3. What is the formula mass of *n*-pentane, C_5H_{12}?

4. What is the formula mass of acetic acid, CH_3CO_2H?

5. What is the formula mass of NaCl?

6. What is the formula mass of KI?

7. How many moles of water are present in 10.0 g H_2O?

8. How many grams of copper(II) nitrate are present in 2.5 moles of $Cu(NO_3)_2$?

9. What is the mass of 1.0×10^{20} carbon atoms?

10. How many atoms are present in 5.0 g of iron?

Medium

1. What is the formula mass of dinitrogen pentoxide?

2. What is the formula mass of xenon tetrafluoride?

3. What is the formula mass of sodium phosphate?

4. What is the formula mass of barium sulfate?

5. How many moles of aluminum nitrate are present in a sample that contains 2.3×10^{26} atoms of O?

6. The medication pravastatin, $C_{23}H_{36}O_7$, is used to control cholesterol levels. What mass of this compound contains 4.8×10^{25} atoms of C?

7. Cisplatin, $Pt(NH_3)_2Cl_2$, is a drug used in chemotherapy. A given sample of cisplatin contains 1.2×10^{24} atoms of Cl. How many grams of cisplatin are present in this sample?

8. Aspirin (also known as acetylsalicylic acid) has the molecular formula $C_9H_8O_4$. If an aspirin tablet contains 4.89×10^{21} atoms of carbon, how many grams of aspirin are in the tablet?

9. Ethanol (C_2H_5OH) is a liquid at room temperature and has a density of 0.789 g/mL. How many moles of ethanol are there in 25.00 mL of ethanol?

10. The density of mercury at room temperature is 13.5 g/mL. How many moles are present in 0.1000 L of mercury?

11. How many moles of ibuprofen are in a 200. mg pill if ibuprofen has the formula $C_{13}H_{18}O_2$?

12. How many molecules of acetaminophen are in two Tylenol pills (325 mg acetaminophen each pill) if acetaminophen has the formula $C_8H_9NO_2$?

Challenge

1. The density of isopropanol, C_3H_8O, is 0.786 g/mL at 20 °C. Determine the volume (in microliters) of isopropanol that contains 3.75×10^{20} atoms of C.

6.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

7: Chemical Equations and Reactions

7.1: Balancing Chemical Equations
7.2: Energy Basics
7.3: Chemical Equilibrium
7.4: Catalysis
7.5: Case Study- Balancing Acts in Pharmacological Synthesis
7.E: Exercises

7: Chemical Equations and Reactions is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

7.1: Balancing Chemical Equations

Learning Objectives

By the end of this section, you will be able to:

- Derive chemical equations from narrative descriptions of chemical reactions.
- Write and balance chemical equations in molecular, total ionic, and net ionic formats.

An earlier chapter of this text introduced the use of element symbols to represent individual atoms. When atoms gain or lose electrons to yield ions, or combine with other atoms to form molecules, their symbols are modified or combined to generate chemical formulas that appropriately represent these species. Extending this symbolism to represent both the identities and the relative quantities of substances undergoing a chemical (or physical) change involves writing and balancing a **chemical equation**. Consider as an example the reaction between one methane molecule (CH_4) and two diatomic oxygen molecules (O_2) to produce one carbon dioxide molecule (CO_2) and two water molecules (H_2O). The chemical equation representing this process is provided in the upper half of Figure **7.1.1**: , with space-filling molecular models shown in the lower half of the figure.

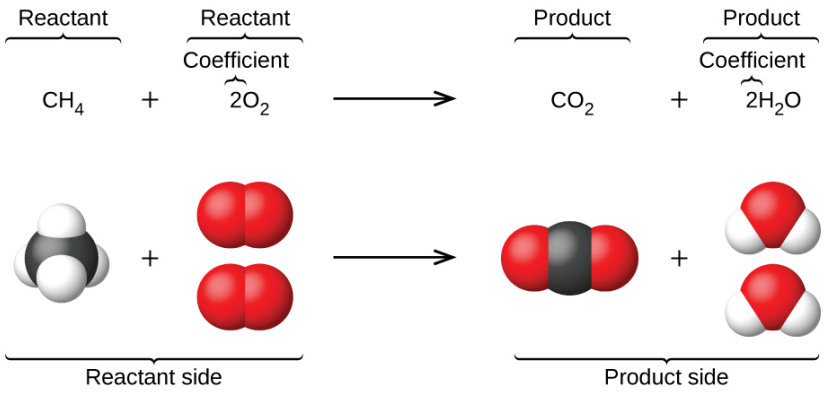


Figure **7.1.1**: The reaction between methane and oxygen to yield carbon dioxide and water (shown at bottom) may be represented by a chemical equation using formulas (top).

This example illustrates the fundamental aspects of any chemical equation:

1. The substances undergoing reaction are called reactants, and their formulas are placed on the left side of the equation.
2. The substances generated by the reaction are called products, and their formulas are placed on the right side of the equation.
3. Plus signs (+) separate individual reactant and product formulas, and an arrow separates the reactant and product (left and right) sides of the equation.
4. The relative numbers of reactant and product species are represented by coefficients (numbers placed immediately to the left of each formula). A coefficient of 1 is typically omitted.

It is common practice to use the smallest possible whole-number coefficients in a chemical equation, as is done in this example. Realize, however, that these coefficients represent the *relative* numbers of reactants and products, and, therefore, they may be correctly interpreted as ratios. Methane and oxygen react to yield carbon dioxide and water in a 1:2:1:2 ratio. This ratio is satisfied if the numbers of these molecules are, respectively, 1-2-1-2, or 2-4-2-4, or 3-6-3-6, and so on (Figure **7.1.2**). Likewise, these coefficients may be interpreted with regard to any amount (number) unit, and so this equation may be correctly read in many ways, including:

- *One* methane molecule and *two* oxygen molecules react to yield *one* carbon dioxide molecule and *two* water molecules.
- *One dozen* methane molecules and *two dozen* oxygen molecules react to yield *one dozen* carbon dioxide molecules and *two dozen* water molecules.
- *One mole* of methane molecules and *2 moles* of oxygen molecules react to yield *1 mole* of carbon dioxide molecules and *2 moles* of water molecules.

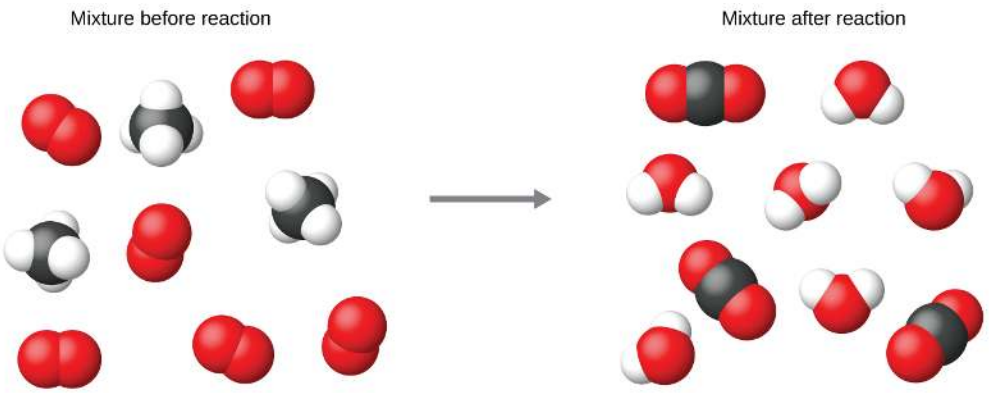


Figure **7.1.2**: Regardless of the absolute numbers of molecules involved, the ratios between numbers of molecules of each species that react (the reactants) and molecules of each species that form (the products) are the same and are given by the chemical reaction equation.

7.1.1: Balancing Equations

The chemical equation described above in Figure **7.1.1** is **balanced**, meaning that equal numbers of atoms for each element involved in the reaction are represented on the reactant and product sides. This is a requirement the equation must satisfy to be consistent with the law of conservation of matter. It may be confirmed by simply summing the numbers of atoms on either side of the arrow and comparing these sums to ensure they are equal. Note that the number of atoms for a given element is calculated by multiplying the coefficient of any formula containing that element by the element's subscript in the formula. If an element appears in more than one formula on a given side of the equation, the number of atoms represented in each must be computed and then added together. For example, both product species in the example reaction, CO_2 and H_2O, contain the element oxygen, and so the number of oxygen atoms on the product side of the equation is

$$\left(1CO_2 \text{ molecule} \times \frac{2O \text{ atoms}}{CO_2 \text{ molecule}}\right) + \left(2H_2O \text{ molecules} \times \frac{1O \text{ atom}}{H_2O \text{ molecule}}\right) = 4O \text{ atoms}$$

The equation for the reaction between methane and oxygen to yield carbon dioxide and water is confirmed to be balanced per this approach, as shown here:

$$\mathrm{CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O}$$

Element	Reactants	Products	Balanced?
C	1 × 1 = 1	1 × 1 = 1	1 = 1, yes
H	4 × 1 = 4	2 × 2 = 4	4 = 4, yes
O	2 × 2 = 4	(1 × 2) + (2 × 1) = 4	4 = 4, yes

A balanced chemical equation often may be derived from a qualitative description of some chemical reaction by a fairly simple approach known as balancing by inspection. Consider as an example the decomposition of water to yield molecular hydrogen and oxygen. This process is represented qualitatively by an *unbalanced* chemical equation:

$$\mathrm{H_2O \longrightarrow H_2 + O_2} \qquad \textbf{(unbalanced)}$$

Comparing the number of **H** and **O** atoms on either side of this equation confirms its imbalance:

Element	Reactants	Products	Balanced?
H	1 × 2 = 2	1 × 2 = 2	2 = 2, yes
O	1 × 1 = 1	1 × 2 = 2	1 ≠ 2, no

The numbers of H atoms on the reactant and product sides of the equation are equal, but the numbers of O atoms are not. To achieve balance, the *coefficients* of the equation may be changed as needed. Keep in mind, of course, that the *formula subscripts* define, in part, the identity of the substance, and so these cannot be changed without altering the qualitative meaning of the equation. For example, changing the reactant formula from H_2O to H_2O_2 would yield balance in the number of atoms, but doing so also changes the reactant's identity (it's now hydrogen peroxide and not water). The O atom balance may be achieved by changing the coefficient for H_2O to 2.

$$\mathbf{2\,H_2O \longrightarrow H_2 + O_2} \qquad \textbf{(unbalanced)}$$

Element	Reactants	Products	Balanced?
H	**2** × 2 = 4	1 × 2 = 2	4 ≠ 2, no
O	2 × 1 = 2	1 × 2 = 2	2 = 2, yes

The H atom balance was upset by this change, but it is easily reestablished by changing the coefficient for the H_2 product to 2.

$$\mathbf{2\,H_2O \longrightarrow 2\,H_2 + O_2} \qquad \textbf{(unbalanced)}$$

Element	Reactants	Products	Balanced?
H	2 × 2 = 4	**2** × 2 = 4	4 = 4, yes
O	2 × 1 = 2	1 × 2 = 2	2 = 2, yes

These coefficients yield equal numbers of both H and O atoms on the reactant and product sides, and the balanced equation is, therefore:

$$\mathbf{H_2O \longrightarrow H_2 + O_2} \qquad \textbf{(balanced)}$$

Example 7.1.1: Balancing Chemical Equations

Write a balanced equation for the reaction of molecular nitrogen (N_2) and oxygen (O_2) to form dinitrogen pentoxide.

Solution

First, write the unbalanced equation.

$$\mathbf{N_2 + O_2 \longrightarrow N_2O_5} \qquad \textbf{(unbalanced)}$$

Next, count the number of each type of atom present in the unbalanced equation.

Element	Reactants	Products	Balanced?
N	1 2 = 2	1 2 = 2	2 = 2, yes
O	1 2 = 2	1 5 = 5	2 ≠ 5, no

Though nitrogen is balanced, changes in coefficients are needed to balance the number of oxygen atoms. To balance the number of oxygen atoms, a reasonable first attempt would be to change the coefficients for the O_2 and N_2O_5 to integers that will yield 10 O atoms (the least common multiple for the O atom subscripts in these two formulas).

$$\mathbf{N_2 + 5\,O_2 \longrightarrow 2\,N_2O_5} \qquad \textbf{(unbalanced)}$$

Element	Reactants	Products	Balanced?
N	1 × 2 = 2	**2** × 2 = 4	2 ≠ 4, no
O	**5** × 2 = 10	**2** × 5 = 10	10 = 10, yes

The N atom balance has been upset by this change; it is restored by changing the coefficient for the reactant N_2 to 2.

$$2\,N_2 + 5\,O_2 \longrightarrow 2\,N_2O_5 \qquad \text{(balanced)}$$

Element	Reactants	Products	Balanced?
N	**2** × 2 = 4	2 × 2 = 4	4 = 4, yes
O	5 × 2 = 10	2 × 5 = 10	10 = 10, yes

The numbers of N and O atoms on either side of the equation are now equal, and so the equation is balanced.

? Exercise 7.1.1

Write a balanced equation for the decomposition of ammonium nitrate to form molecular nitrogen, molecular oxygen, and water. (Hint: Balance oxygen last, since it is present in more than one molecule on the right side of the equation.)

Answer

$$2\,NH_4NO_3 \longrightarrow 2\,N_2 = O_2 + 4\,H_2O$$

It is sometimes convenient to use fractions instead of integers as intermediate coefficients in the process of balancing a chemical equation. When balance is achieved, all the equation's coefficients may then be multiplied by a whole number to convert the fractional coefficients to integers without upsetting the atom balance. For example, consider the reaction of ethane (C_2H_6) with oxygen to yield H_2O and CO_2, represented by the unbalanced equation:

$$C_2H_6 + O_2 \longrightarrow H_2O + CO_2 \qquad \text{(unbalanced)}$$

Following the usual inspection approach, one might first balance C and H atoms by changing the coefficients for the two product species, as shown:

$$C_2H_6 + O_2 \longrightarrow 3\,H_2O + 2\,CO_2 \qquad \text{(unbalanced)}$$

This results in seven O atoms on the product side of the equation, an odd number—no integer coefficient can be used with the O_2 reactant to yield an odd number, so a fractional coefficient, is used instead to yield a provisional balanced equation:

$$C_2H_6 + \tfrac{7}{2}\,O_2 \longrightarrow 3\,H_2O + 2\,CO_2 \qquad \text{(unbalanced)}$$

A conventional balanced equation with integer-only coefficients is derived by multiplying each coefficient by 2:

$$2\,C_2H_6 + 7\,O_2 \longrightarrow 6\,H_2O + 4\,CO_2 \qquad \text{(balanced)}$$

Finally with regard to balanced equations, recall that convention dictates use of the *smallest whole-number coefficients*. Although the equation for the reaction between molecular nitrogen and molecular hydrogen to produce ammonia is, indeed, balanced,

$$3\,N_2 + 9\,H_2 \longrightarrow 6\,NH_3$$

the coefficients are not the smallest possible integers representing the relative numbers of reactant and product molecules. Dividing each coefficient by the greatest common factor, 3, gives the preferred equation:

$$N_2 + 3\,H_2 \longrightarrow 2\,NH_3$$

Link to Learning

Use this interactive tutorial for additional practice balancing equations.

7.1.2: Additional Information in Chemical Equations

The physical states of reactants and products in chemical equations very often are indicated with a parenthetical abbreviation following the formulas. Common abbreviations include *s* for solids, *l* for liquids, *g* for gases, and *aq* for substances dissolved in

water (*aqueous solutions*, as introduced in the preceding chapter). These notations are illustrated in the example equation here:

$$2\,Na\,(s) + 2\,H_2O\,(l) \longrightarrow 2\,NaOH\,(aq) + H_2\,(g)$$

This equation represents the reaction that takes place when sodium metal is placed in water. The solid sodium reacts with liquid water to produce molecular hydrogen gas and the ionic compound sodium hydroxide (a solid in pure form, but readily dissolved in water).

Special conditions necessary for a reaction are sometimes designated by writing a word or symbol above or below the equation's arrow. For example, a reaction carried out by heating may be indicated by the uppercase Greek letter delta (Δ) over the arrow.

$$CaCO_3\,(s) \xrightarrow{\Delta} CaO\,(s) + CO_2\,(g)$$

Other examples of these special conditions will be encountered in more depth in later chapters.

7.1.3: Equations for Ionic Reactions

Given the abundance of water on earth, it stands to reason that a great many chemical reactions take place in aqueous media. When ions are involved in these reactions, the chemical equations may be written with various levels of detail appropriate to their intended use. To illustrate this, consider a reaction between ionic compounds taking place in an aqueous solution. When aqueous solutions of $CaCl_2$ and $AgNO_3$ are mixed, a reaction takes place producing aqueous $Ca(NO_3)_2$ and solid AgCl:

$$CaCl_2\,(aq) + 2\,AgNO_3\,(aq) \longrightarrow Ca(NO_3)_2\,(aq) + 2\,AgCl\,(s)$$

This balanced equation, derived in the usual fashion, is called a **molecular equation** because it doesn't explicitly represent the ionic species that are present in solution. When ionic compounds dissolve in water, they may *dissociate* into their constituent ions, which are subsequently dispersed homogenously throughout the resulting solution (a thorough discussion of this important process is provided in the chapter on solutions). Ionic compounds dissolved in water are, therefore, more realistically represented as dissociated ions, in this case:

$$CaCl_2\,(aq) \longrightarrow Ca^{2+}\,(aq) + 2\,Cl^-\,(aq)$$
$$2\,AgNO_3\,(aq) \longrightarrow 2\,Ag^+\,(aq) + 2\,NO_3{}^-\,(aq)$$
$$Ca(NO_3)_2\,(aq) \longrightarrow Ca^{2+}\,(aq) + 2\,NO_3{}^-\,(aq)$$

Unlike these three ionic compounds, AgCl does not dissolve in water to a significant extent, as signified by its physical state notation, *s*.

Explicitly representing all dissolved ions results in a **complete ionic equation**. In this particular case, the formulas for the dissolved ionic compounds are replaced by formulas for their dissociated ions:

$$Ca^{2+}\,(aq) + 2\,Cl^-\,(aq) + 2\,Ag^+\,(aq) + 2\,NO_3{}^-\,(aq) \longrightarrow Ca^{2+}\,(aq) + 2\,NO_3{}^-\,(aq) + 2\,AgCl\,(s)$$

Examining this equation shows that two chemical species are present in identical form on both sides of the arrow, $Ca^{2+}(aq)$ and These spectator ions—ions whose presence is required to maintain charge neutrality—are neither chemically nor physically changed by the process, and so they may be eliminated from the equation to yield a more succinct representation called a **net ionic equation**:

$$\cancel{Ca^{2+}\,(aq)} + 2\,Cl^-\,(aq) + 2\,Ag^+\,(aq) + \cancel{2NO3^-\,(aq)} \longrightarrow \cancel{Ca^{2+}\,(aq)} + \cancel{2NO3^-\,(aq)} + 2\,AgCl\,(s)$$
$$2\,Cl^-\,(aq) + 2\,Ag^+\,(aq) \longrightarrow 2\,AgCl\,(s)$$

Following the convention of using the smallest possible integers as coefficients, this equation is then written:

$$Cl^-\,(aq) + Ag^+\,(aq) \longrightarrow AgCl\,(s)$$

This net ionic equation indicates that solid silver chloride may be produced from dissolved chloride and silver(I) ions, regardless of the source of these ions. These molecular and complete ionic equations provide additional information, namely, the ionic compounds used as sources of Cl^- and Ag^+.

Example 7.1.2: Ionic and Molecular Equations

When carbon dioxide is dissolved in an aqueous solution of sodium hydroxide, the mixture reacts to yield aqueous sodium carbonate and liquid water. Write balanced molecular, complete ionic, and net ionic equations for this process.

Solution

Begin by identifying formulas for the reactants and products and arranging them properly in chemical equation form:

$$\mathrm{CO_2\,(aq) + NaOH\,(aq) \longrightarrow Na_2CO_3\,(aq) + H_2O\,(l)} \qquad \text{(unbalanced)}$$

Balance is achieved easily in this case by changing the coefficient for NaOH to 2, resulting in the molecular equation for this reaction:

$$\mathrm{CO_2\,(aq) + 2\,NaOH\,(aq) \longrightarrow Na_2CO_3\,(aq) + H_2O\,(l)}$$

The two dissolved ionic compounds, NaOH and $\mathrm{Na_2CO_3}$, can be represented as dissociated ions to yield the complete ionic equation:

$$\mathrm{CO_2\,(aq) + 2\,Na^+\,(aq) + OH^-\,(aq) \longrightarrow 2\,Na^+\,(aq) + CO_3^{2-}\,(aq) + H_2O\,(l)}$$

Finally, identify the spectator ion(s), in this case $\mathrm{Na^+}(aq)$, and remove it from each side of the equation to generate the net ionic equation:

$$\mathrm{CO_2\,(aq) + \cancel{2Na^+\,(aq)} + OH^-\,(aq) \longrightarrow \cancel{2Na^+\,(aq)} + CO_3^{2-}\,(aq) + H_2O\,(l)}$$

$$\mathrm{CO_2\,(aq) + OH^-\,(aq) \longrightarrow CO_3^{2-}\,(aq) + H_2O\,(l)}$$

Exercise 7.1.2

Diatomic chlorine and sodium hydroxide (lye) are commodity chemicals produced in large quantities, along with diatomic hydrogen, via the electrolysis of brine, according to the following unbalanced equation:

$$\mathrm{NaCl\,(aq) + H_2O\,(l) \xrightarrow{electricity} NaOH\,(aq) + H_2\,(g) + Cl_2\,(g)}$$

Write balanced molecular, complete ionic, and net ionic equations for this process.

Answer

$$\mathrm{2\,NaCl\,(aq) + 2\,H_2O\,(l) \longrightarrow 2\,NaOH\,(aq) + H_2\,(g) + Cl_2\,(g)} \qquad \text{(molecular)}$$

$$\mathrm{2\,Na^+\,(aq) + 2\,Cl^-\,(aq) + 2\,H_2O\,(l) \longrightarrow 2\,Na^+\,(aq) + 2\,OH^-\,(aq) + H_2\,(g) + Cl_2\,(g)} \qquad \text{(complete ionic)}$$

$$\mathrm{2\,Cl^-\,(aq) + 2\,H_2O\,(l) \longrightarrow 2\,OH^-\,(aq) + H_2\,(g) + Cl_2\,(g)} \qquad \text{(net ionic)}$$

This page titled 7.1: Balancing Chemical Equations is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

7.2: Energy Basics

Learning Objectives

By the end of this section, you will be able to:

- Define energy, distinguish types of energy, and describe the nature of energy changes that accompany chemical and physical changes
- Distinguish the related properties of heat, thermal energy, and temperature
- Define and distinguish specific heat and heat capacity, and describe the physical implications of both
- Perform calculations involving heat, specific heat, and temperature change

Chemical changes and their accompanying changes in energy are important parts of our everyday world (Figure **7.2.1**). The macronutrients in food (proteins, fats, and carbohydrates) undergo metabolic reactions that provide the energy to keep our bodies functioning. We burn a variety of fuels (gasoline, natural gas, coal) to produce energy for transportation, heating, and the generation of electricity. Industrial chemical reactions use enormous amounts of energy to produce raw materials (such as iron and aluminum). Energy is then used to manufacture those raw materials into useful products, such as cars, skyscrapers, and bridges.



(a) (b) (c)

Figure **7.2.1**: The energy involved in chemical changes is important to our daily lives: (a) A cheeseburger for lunch provides the energy you need to get through the rest of the day; (b) the combustion of gasoline provides the energy that moves your car (and you) between home, work, and school; and (c) coke, a processed form of coal, provides the energy needed to convert iron ore into iron, which is essential for making many of the products we use daily. (credit a: modification of work by "Pink Sherbet Photography"/Flickr; credit b: modification of work by Jeffery Turner)

Over 90% of the energy we use comes originally from the sun. Every day, the sun provides the earth with almost 10,000 times the amount of energy necessary to meet all of the world's energy needs for that day. Our challenge is to find ways to convert and store incoming solar energy so that it can be used in reactions or chemical processes that are both convenient and nonpolluting. Plants and many bacteria capture solar energy through photosynthesis. We release the energy stored in plants when we burn wood or plant products such as ethanol. We also use this energy to fuel our bodies by eating food that comes directly from plants or from animals that got their energy by eating plants. Burning coal and petroleum also releases stored solar energy: These fuels are fossilized plant and animal matter.

This chapter will introduce the basic ideas of an important area of science concerned with the amount of heat absorbed or released during chemical and physical changes—an area called thermochemistry. The concepts introduced in this chapter are widely used in almost all scientific and technical fields. Food scientists use them to determine the energy content of foods. Biologists study the energetics of living organisms, such as the metabolic combustion of sugar into carbon dioxide and water. The oil, gas, and transportation industries, renewable energy providers, and many others endeavor to find better methods to produce energy for our commercial and personal needs. Engineers strive to improve energy efficiency, find better ways to heat and cool our homes, refrigerate our food and drinks, and meet the energy and cooling needs of computers and electronics, among other applications. Understanding thermochemical principles is essential for chemists, physicists, biologists, geologists, every type of engineer, and just about anyone who studies or does any kind of science.

7.2.1: Energy

Energy can be defined as the capacity to supply heat or do work. One type of work (w) is the process of causing matter to move against an opposing force. For example, we do work when we inflate a bicycle tire—we move matter (the air in the pump) against

the opposing force of the air already in the tire.

Like matter, energy comes in different types. One scheme classifies energy into two types: potential energy, the energy an object has because of its relative position, composition, or condition, and kinetic energy, the energy that an object possesses because of its motion. Water at the top of a waterfall or dam has potential energy because of its position; when it flows downward through generators, it has kinetic energy that can be used to do work and produce electricity in a hydroelectric plant (Figure **7.2.2**). A battery has potential energy because the chemicals within it can produce electricity that can do work.



(a) (b)

Figure **7.2.2**: (a) Water at a higher elevation, for example, at the top of Victoria Falls, has a higher potential energy than water at a lower elevation. As the water falls, some of its potential energy is converted into kinetic energy. (b) If the water flows through generators at the bottom of a dam, such as the Hoover Dam shown here, its kinetic energy is converted into electrical energy. (credit a: modification of work by Steve Jurvetson; credit b: modification of work by "curimedia"/Wikimedia commons)

Energy can be converted from one form into another, but all of the energy present before a change occurs always exists in some form after the change is completed. This observation is expressed in the law of conservation of energy: during a chemical or physical change, energy can be neither created nor destroyed, although it can be changed in form. (This is also one version of the first law of thermodynamics, as you will learn later.)

When one substance is converted into another, there is always an associated conversion of one form of energy into another. Heat is usually released or absorbed, but sometimes the conversion involves light, electrical energy, or some other form of energy. For example, chemical energy (a type of potential energy) is stored in the molecules that compose gasoline. When gasoline is combusted within the cylinders of a car's engine, the rapidly expanding gaseous products of this chemical reaction generate mechanical energy (a type of kinetic energy) when they move the cylinders' pistons.

According to the law of conservation of matter (seen in an earlier chapter), there is no detectable change in the total amount of matter during a chemical change. When chemical reactions occur, the energy changes are relatively modest and the mass changes are too small to measure, so the laws of conservation of matter and energy hold well. However, in nuclear reactions, the energy changes are much larger (by factors of a million or so), the mass changes are measurable, and matter-energy conversions are significant. This will be examined in more detail in a later chapter on nuclear chemistry.

7.2.2: Thermal Energy, Temperature, and Heat

Thermal energy is kinetic energy associated with the random motion of atoms and molecules. Temperature is a quantitative measure of "hot" or "cold." When the atoms and molecules in an object are moving or vibrating quickly, they have a higher average kinetic energy (KE), and we say that the object is "hot." When the atoms and molecules are moving slowly, they have lower average KE, and we say that the object is "cold" (Figure **7.2.3**). Assuming that no chemical reaction or phase change (such as melting or vaporizing) occurs, increasing the amount of thermal energy in a sample of matter will cause its temperature to increase. And, assuming that no chemical reaction or phase change (such as condensation or freezing) occurs, decreasing the amount of thermal energy in a sample of matter will cause its temperature to decrease.

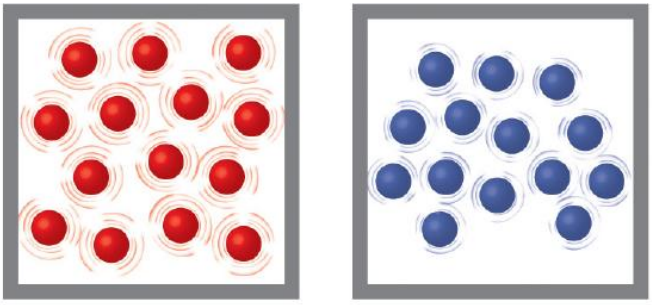


Figure **7.2.3**: (a) The molecules in a sample of hot water move more rapidly than (b) those in a sample of cold water.

Link to Learning

Click on this interactive simulation to view the effects of temperature on molecular motion.

Most substances expand as their temperature increases and contract as their temperature decreases. This property can be used to measure temperature changes, as shown in Figure **7.2.4**. The operation of many thermometers depends on the expansion and contraction of substances in response to temperature changes.

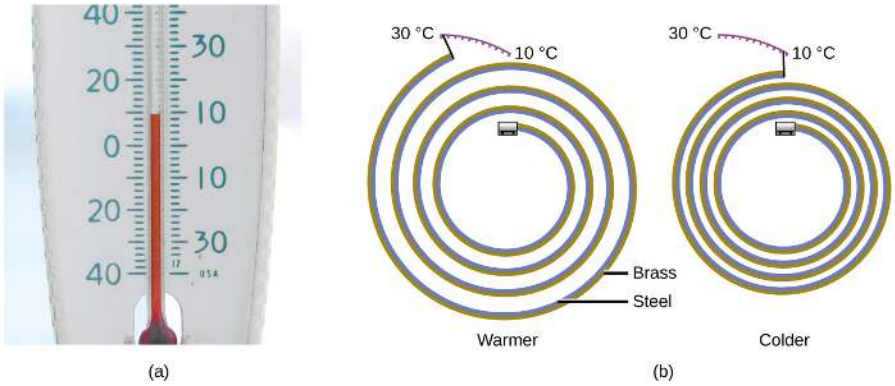


Figure **7.2.4**: (a) In an alcohol or mercury thermometer, the liquid (dyed red for visibility) expands when heated and contracts when cooled, much more so than the glass tube that contains the liquid. (b) In a bimetallic thermometer, two different metals (such as brass and steel) form a two-layered strip. When heated or cooled, one of the metals (brass) expands or contracts more than the other metal (steel), causing the strip to coil or uncoil. Both types of thermometers have a calibrated scale that indicates the temperature. (credit a: modification of work by “dwstucke”/Flickr)

Link to Learning

The following demonstration allows one to view the effects of heating and cooling a coiled bimetallic strip.

Heat (q) is the transfer of thermal energy between two bodies at different temperatures. Heat flow (a redundant term, but one commonly used) increases the thermal energy of one body and decreases the thermal energy of the other. Suppose we initially have a high temperature (and high thermal energy) substance (H) and a low temperature (and low thermal energy) substance (L). The atoms and molecules in H have a higher average KE than those in L. If we place substance H in contact with substance L, the thermal energy will flow spontaneously from substance H to substance L. The temperature of substance H will decrease, as will the average KE of its molecules; the temperature of substance L will increase, along with the average KE of its molecules. Heat flow will continue until the two substances are at the same temperature (Figure **7.2.5**).

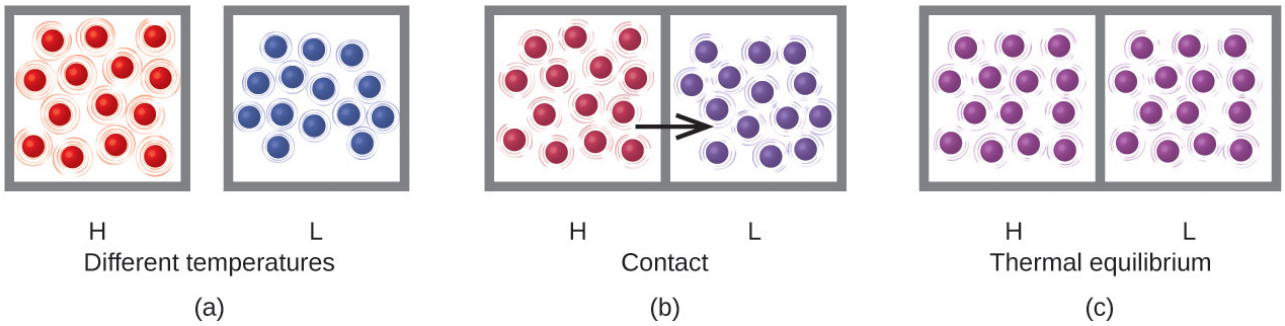


Figure **7.2.5**: (a) Substances H and L are initially at different temperatures, and their atoms have different average kinetic energies. (b) When they contact each other, collisions between the molecules result in the transfer of kinetic (thermal) energy from the hotter to the cooler matter. (c) The two objects reach "thermal equilibrium" when both substances are at the same temperature and their molecules have the same average kinetic energy.

Link to Learning

Click on the PhET simulation to explore energy forms and changes. Visit the Energy Systems tab to create combinations of energy sources, transformation methods, and outputs. Click on Energy Symbols to visualize the transfer of energy.

Matter undergoing chemical reactions and physical changes can release or absorb heat. A change that releases heat is called an exothermic process. For example, the combustion reaction that occurs when using an oxyacetylene torch is an exothermic process—this process also releases energy in the form of light as evidenced by the torch's flame (Figure **7.2.6**). A reaction or change that absorbs heat is an endothermic process. A cold pack used to treat muscle strains provides an example of an endothermic process. When the substances in the cold pack (water and a salt like ammonium nitrate) are brought together, the resulting process absorbs heat, leading to the sensation of cold.



Figure **7.2.6**: (a) An oxyacetylene torch produces heat by the combustion of acetylene in oxygen. The energy released by this exothermic reaction heats and then melts the metal being cut. The sparks are tiny bits of the molten metal flying away. (b) A cold pack uses an endothermic process to create the sensation of cold. (credit a: modification of work by "Skatebiker"/Wikimedia commons)

Historically, energy was measured in units of calories (cal). A calorie is the amount of energy required to raise one gram of water by 1 degree C (1 kelvin). However, this quantity depends on the atmospheric pressure and the starting temperature of the water. The ease of measurement of energy changes in calories has meant that the calorie is still frequently used. The Calorie (with a capital C), or large calorie, commonly used in quantifying food energy content, is a kilocalorie. The SI unit of heat, work, and energy is the joule. A joule (J) is defined as the amount of energy used when a force of 1 newton moves an object 1 meter. It is named in honor of the English physicist James Prescott Joule. One joule is equivalent to 1 kg m^2/s^2, which is also called 1 newton–meter. A kilojoule (kJ) is 1000 joules. To standardize its definition, 1 calorie has been set to equal 4.184 joules.

We now introduce two concepts useful in describing heat flow and temperature change. The heat capacity (C) of a body of matter is the quantity of heat (q) it absorbs or releases when it experiences a temperature change (ΔT) of 1 degree Celsius (or equivalently, 1 kelvin):

$$C = \frac{q}{\Delta T}$$

Heat capacity is determined by both the type and amount of substance that absorbs or releases heat. It is therefore an extensive property—its value is proportional to the amount of the substance.

For example, consider the heat capacities of two cast iron frying pans. The heat capacity of the large pan is five times greater than that of the small pan because, although both are made of the same material, the mass of the large pan is five times greater than the mass of the small pan. More mass means more atoms are present in the larger pan, so it takes more energy to make all of those atoms vibrate faster. The heat capacity of the small cast iron frying pan is found by observing that it takes 18,150 J of energy to raise the temperature of the pan by 50.0 °C:

$$C_{\text{small pan}} = \frac{18,140J}{50.0°C} = 363J/°C$$

The larger cast iron frying pan, while made of the same substance, requires 90,700 J of energy to raise its temperature by 50.0 °C. The larger pan has a (proportionally) larger heat capacity because the larger amount of material requires a (proportionally) larger amount of energy to yield the same temperature change:

$$C_{\text{large pan}} = \frac{90,700J}{50.0°C} = 1814J/°C$$

The specific heat capacity (*c*) of a substance, commonly called its "specific heat," is the quantity of heat required to raise the temperature of 1 gram of a substance by 1 degree Celsius (or 1 kelvin):

$$c = \frac{q}{m\Delta T}$$

Specific heat capacity depends only on the kind of substance absorbing or releasing heat. It is an intensive property—the type, but not the amount, of the substance is all that matters. For example, the small cast iron frying pan has a mass of 808 g. The specific heat of iron (the material used to make the pan) is therefore:

$$c_{\text{iron}} = \frac{18,140J}{(808g)\,(50.0°C)} = 0.449J/g°C$$

The large frying pan has a mass of 4040 g. Using the data for this pan, we can also calculate the specific heat of iron:

$$c_{\text{iron}} = \frac{90,700J}{(4040g)\,(50.0°C)} = 0.449J/g°C$$

Although the large pan is more massive than the small pan, since both are made of the same material, they both yield the same value for specific heat (for the material of construction, iron). Note that specific heat is measured in units of energy per temperature per mass and is an intensive property, being derived from a ratio of two extensive properties (heat and mass). The molar heat capacity, also an intensive property, is the heat capacity per mole of a particular substance and has units of J/mol °C (Figure **7.2.7**).



Figure **7.2.7**: Because of its larger mass, a large frying pan has a larger heat capacity than a small frying pan. Because they are made of the same material, both frying pans have the same specific heat. (credit: Mark Blaser)

Water has a relatively high specific heat (about 4.2 J/g °C for the liquid and 2.09 J/g °C for the solid); most metals have much lower specific heats (usually less than 1 J/g °C). The specific heat of a substance varies somewhat with temperature. However, this

variation is usually small enough that we will treat specific heat as constant over the range of temperatures that will be considered in this chapter. Specific heats of some common substances are listed in Table **7.2.1**.

Table **7.2.1**: Specific Heats of Common Substances at 25 °C and 1 bar

Substance	Symbol (*state*)	Specific Heat (J/g °C)
helium	$He(g)$	5.193
water	$H_2O(l)$	4.184
ethanol	$C_2H_6O(l)$	2.376
ice	$H_2O(s)$	2.093 (at −10 °C)
water vapor	$H_2O(g)$	1.864
nitrogen	$N_2(g)$	1.040
air		1.007
oxygen	$O_2(g)$	0.918
aluminum	$Al(s)$	0.897
carbon dioxide	$CO_2(g)$	0.853
argon	$Ar(g)$	0.522
iron	$Fe(s)$	0.449
copper	$Cu(s)$	0.385
lead	$Pb(s)$	0.130
gold	$Au(s)$	0.129
silicon	$Si(s)$	0.712

If we know the mass of a substance and its specific heat, we can determine the amount of heat, q, entering or leaving the substance by measuring the temperature change before and after the heat is gained or lost:

$$\begin{aligned} q &= (\text{ specific heat }) \times (\text{ mass of substance }) \times (\text{ temperature change }) \\ &= c \times m \times \Delta T \\ &= c \times m \times (T_{\text{final}} - T_{\text{initial}}) \end{aligned} \tag{7.2.1}$$

In this equation, c is the specific heat of the substance, m is its mass, and ΔT (which is read “delta T”) is the temperature change, $T_{\text{final}} - T_{\text{initial}}$. If a substance gains thermal energy, its temperature increases, its final temperature is higher than its initial temperature, $T_{\text{final}} - T_{\text{initial}}$ has a positive value, and the value of q is positive. If a substance loses thermal energy, its temperature decreases, the final temperature is lower than the initial temperature, $T_{\text{final}} - T_{\text{initial}}$ has a negative value, and the value of q is negative.

✔ Example 7.2.1: Measuring Heat

A flask containing 8.0 10^2 g of water is heated, and the temperature of the water increases from 21 °C to 85 °C. How much heat did the water absorb?

Solution

To answer this question, consider these factors:

- the specific heat of the substance being heated (in this case, water)
- the amount of substance being heated (in this case, 8.0×10^2 g)

- the magnitude of the temperature change (in this case, from 21 °C to 85 °C).

The specific heat of water is 4.184 J/g °C, so to heat 1 g of water by 1 °C requires 4.184 J. We note that since 4.184 J is required to heat 1 g of water by 1 °C, we will need *800 times as much* to heat 8.0×10^2 g of water by 1 °C. Finally, we observe that since 4.184 J are required to heat 1 g of water by 1 °C, we will need *64 times as much* to heat it by 64 °C (that is, from 21 °C to 85 °C).

This can be summarized using Equation 7.2.1:

$$\begin{aligned} q &= c \times m \times \Delta T = c \times m \times (T_{\text{final}} - T_{\text{initial}}) \\ &= \left(4.184 J/\frac{g}{\circ}°C\right) \times (8.0 \times 10^2 g) \times (85 - 21)°C \\ &= (4.184 J/g°C) \times (8.0 \times 10^2 g) \times (64)°C \\ &= 210,000 J \left(= 2.1 \times 10^2 kJ\right) \end{aligned} \tag{7.2.2}$$

Because the temperature increased, the water absorbed heat and q is positive.

? Exercise 7.2.1

How much heat, in joules, must be added to a 502 g iron skillet to increase its temperature from 25 °C to 250 °C? The specific heat of iron is 0.449 J/g °C.

Answer

$5.07\ 10^4$ J

Note that the relationship between heat, specific heat, mass, and temperature change can be used to determine any of these quantities (not just heat) if the other three are known or can be deduced.

✓ Example 7.2.2: Determining Other Quantities

A piece of unknown metal weighs 348 g. When the metal piece absorbs 6.64 kJ of heat, its temperature increases from 22.4 °C to 43.6 °C. Determine the specific heat of this metal (which might provide a clue to its identity).

Solution

Since mass, heat, and temperature change are known for this metal, we can determine its specific heat using the relationship in Equation 7.2.1:

$$q = c \times m \times \Delta T = c \times m \times (T_{\text{final}} - T_{\text{initial}})$$

Substituting the known values:

$$6640 J = c \times (348 g) \times (43.6 - 22.4)°C$$

Solving:

$$c = \frac{6640 J}{(348 g) \times (21.2°C)} = 0.900 J/g°C$$

Comparing this value with the values in Table 7.2.1, this value matches the specific heat of aluminum, which suggests that the unknown metal may be aluminum.

? Exercise 7.2.2

A piece of unknown metal weighs 217 g. When the metal piece absorbs 1.43 kJ of heat, its temperature increases from 24.5 °C to 39.1 °C. Determine the specific heat of this metal, and predict its identity.

Answer

c = 0.451 J/g °C; the metal is likely to be iron

Chemistry in Everyday Life: Solar Thermal Energy Power Plants

The sunlight that reaches the earth contains thousands of times more energy than we presently capture. Solar thermal systems provide one possible solution to the problem of converting energy from the sun into energy we can use. Large-scale solar thermal plants have different design specifics, but all concentrate sunlight to heat some substance; the heat "stored" in that substance is then converted into electricity.

The Solana Generating Station in Arizona's Sonora Desert produces 280 megawatts of electrical power. It uses parabolic mirrors that focus sunlight on pipes filled with a heat transfer fluid (HTF) (Figure **7.2.8**). The HTF then does two things: It turns water into steam, which spins turbines, which in turn produces electricity, and it melts and heats a mixture of salts, which functions as a thermal energy storage system. After the sun goes down, the molten salt mixture can then release enough of its stored heat to produce steam to run the turbines for 6 hours. Molten salts are used because they possess a number of beneficial properties, including high heat capacities and thermal conductivities.

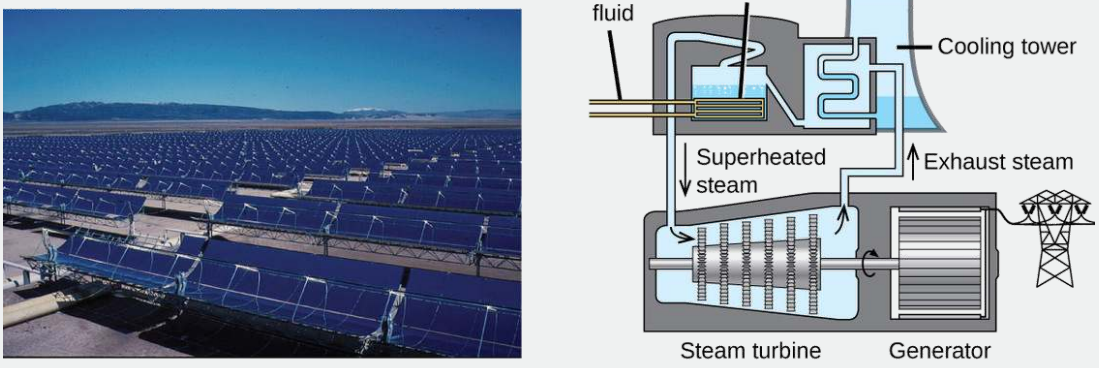


Figure **7.2.8**: This solar thermal plant uses parabolic trough mirrors to concentrate sunlight. (credit a: modification of work by Bureau of Land Management)

The 377-megawatt Ivanpah Solar Generating System, located in the Mojave Desert in California, is the largest solar thermal power plant in the world (Figure **7.2.9**). Its 170,000 mirrors focus huge amounts of sunlight on three water-filled towers, producing steam at over 538 °C that drives electricity-producing turbines. It produces enough energy to power 140,000 homes. Water is used as the working fluid because of its large heat capacity and heat of vaporization.



Figure **7.2.9**: (a) The Ivanpah solar thermal plant uses 170,000 mirrors to concentrate sunlight on water-filled towers. (b) It covers 4000 acres of public land near the Mojave Desert and the California-Nevada border. (credit a: modification of work by Craig Dietrich; credit b: modification of work by "USFWS Pacific Southwest Region"/Flickr)

This page titled 7.2: Energy Basics is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **5.1: Energy Basics** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

7.3: Chemical Equilibrium

Learning Objectives

- Describe the ways in which an equilibrium system can be stressed
- Predict the response of a stressed equilibrium using Le Chatelier's principle

As we saw in the previous section, reactions proceed in both directions (reactants go to products and products go to reactants). We can tell a reaction is at equilibrium if the reaction quotient (Q) is equal to the equilibrium constant (K). We next address what happens when a system at equilibrium is disturbed so that Q is no longer equal to K. If a system at equilibrium is subjected to a perturbance or stress (such as a change in concentration) the position of equilibrium changes. Since this stress affects the concentrations of the reactants and the products, the value of Q will no longer equal the value of K. To re-establish equilibrium, the system will either shift toward the products (if ($Q \leq K$) or the reactants (if ($Q \geq K$) until Q returns to the same value as K. This process is described by Le Chatelier's principle.

Le Chatelier's principle

When a chemical system at equilibrium is disturbed, it returns to equilibrium by counteracting the disturbance. As described in the previous paragraph, the disturbance causes a change in Q; the reaction will shift to re-establish $Q = K$.

Predicting the Direction of a Reversible Reaction

Le Chatelier's principle can be used to predict changes in equilibrium concentrations when a system that is at equilibrium is subjected to a stress. However, if we have a mixture of reactants and products that have not yet reached equilibrium, the changes necessary to reach equilibrium may not be so obvious. In such a case, we can compare the values of Q and K for the system to predict the changes.

> *A chemical system at equilibrium can be **temporarily** shifted out of equilibrium by adding or removing one or more of the reactants or products. The concentrations of both reactants and products then undergo additional changes to return the system to equilibrium.*

The stress on the system in Figure **7.3.1** is the reduction of the equilibrium concentration of SCN^- (lowering the concentration of one of the reactants would cause Q to be larger than K). As a consequence, Le Chatelier's principle leads us to predict that the concentration of $Fe(SCN)^{2+}$ should decrease, increasing the concentration of SCN^- part way back to its original concentration, and increasing the concentration of Fe^{3+} above its initial equilibrium concentration.



Figure **7.3.1**: (a) The test tube contains 0.1 M Fe^{3+}. (b) Thiocyanate ion has been added to solution in (a), forming the red $Fe(SCN)^{2+}$ ion. $\mathbf{Fe^{3+}(aq) + SCN^-(aq) \rightleftharpoons Fe(SCN)^{2+}(aq)}$. (c) Silver nitrate has been added to the solution in (b), precipitating some of the SCN− as the white solid AgSCN. $\mathbf{Ag^+(aq) + SCN^-(aq) \rightleftharpoons AgSCN(s)}$. The decrease in the SCN− concentration shifts the first equilibrium in the solution to the left, decreasing the concentration (and lightening color) of the $Fe(SCN)^{2+}$. (credit: modification of work by Mark Ott).

The effect of a change in concentration on a system at equilibrium is illustrated further by the equilibrium of this chemical reaction:

$$\mathrm{H_2(g) + I_2(g) \rightleftharpoons 2\,HI(g)} \tag{7.3.1}$$

$$K_c = 50.0 \text{ at } 400^\circ\mathrm{C} \tag{7.3.2}$$

The numeric values for this example have been determined experimentally. A mixture of gases at 400 °C with $[\mathrm{H_2}] = [\mathrm{I_2}] = 0.221\ M$ and $[\mathrm{HI}] = 1.563\ M$ is at equilibrium; for this mixture, $Q_c = K_c = 50.0$. If $\mathrm{H_2}$ is introduced into the system so quickly that its concentration doubles before it begins to react (new $[\mathrm{H_2}] = 0.442\ M$), the reaction will shift so that a new equilibrium is reached, at which

- $[\mathrm{H_2}] = 0.374\ M$,
- $[\mathrm{I_2}] = 0.153\ M$, and
- $[\mathrm{HI}] = 1.692\ M$.

This gives:

$$\begin{aligned} Q_c &= \frac{[\mathrm{HI}]^2}{[\mathrm{H_2}][\mathrm{I_2}]} \\ &= \frac{(1.692)^2}{(0.374)(0.153)} \\ &= 50.0 = K_c \end{aligned}$$

We have stressed this system by introducing additional $\mathrm{H_2}$. The stress is relieved when the reaction shifts to the right, using up some (but not all) of the excess $\mathrm{H_2}$, reducing the amount of uncombined $\mathrm{I_2}$, and forming additional HI. **Le Chatelier's Principle (Changing Concentrations):** Le Chatelier's Principle (Changing Concentrations)(opens in new window) [youtu.be]



A Video Discussing Le Chatelier's Principle (Changing Concentrations): Le Chatelier's Principle (Changing Concentrations)(opens in new window) [youtu.be] (opens in new window)

Effect of Change in Pressure on Equilibrium

Sometimes we can change the position of equilibrium by changing the pressure of a system. However, changes in pressure have a measurable effect only in systems in which gases are involved, and then only when the chemical reaction produces a change in the total number of gas molecules in the system. An easy way to recognize such a system is to look for different numbers of moles of gas on the reactant and product sides of the equilibrium. While evaluating pressure (as well as related factors like volume), it is important to remember that equilibrium constants are defined with regard to concentration (for K_c) or partial pressure (for K_P). Some changes to total pressure, like adding an inert gas that is not part of the equilibrium, will change the total pressure but not the partial pressures of the gases in the equilibrium constant expression. Thus, addition of a gas not involved in the equilibrium will not perturb the equilibrium.

As we increase the pressure of a gaseous system at equilibrium, either by decreasing the volume of the system or by adding more of one of the components of the equilibrium mixture, we introduce a stress by increasing the partial pressures of one or more of the

components. In accordance with Le Chatelier's principle, a shift in the equilibrium that reduces the total number of molecules per unit of volume will be favored because this relieves the stress. The reverse reaction would be favored by a decrease in pressure.

Consider what happens when we increase the pressure on a system in which NO, $\mathrm{O_2}$, and $\mathrm{NO_2}$ are at equilibrium:

$$2\,\mathrm{NO}\,(g) + \mathrm{O_2}\,(g) \rightleftharpoons 2\,\mathrm{NO_2}\,(g) \tag{7.3.3}$$

The formation of additional amounts of $\mathrm{NO_2}$ decreases the total number of molecules in the system because each time two molecules of $\mathrm{NO_2}$ form, a total of three molecules of NO and $\mathrm{O_2}$ are consumed. This reduces the total pressure exerted by the system and reduces, but does not completely relieve, the stress of the increased pressure. On the other hand, a decrease in the pressure on the system favors decomposition of $\mathrm{NO_2}$ into NO and $\mathrm{O_2}$, which tends to restore the pressure.

Now consider this reaction:

$$\mathrm{N_2}\,(g) + \mathrm{O_2}\,(g) \rightleftharpoons 2\,\mathrm{NO}\,(g) \tag{7.3.4}$$

Because there is no change in the total number of molecules in the system during reaction, a change in pressure does not favor either formation or decomposition of gaseous nitrogen monoxide.



Le Chatelier’s Principle (Changes in Pressure or Volume):

Le Chatelier’s Principle (Changes in Pressure or Volume)(opens in new window) [youtu.be]

Effect of Change in Temperature on Equilibrium

Changing concentration or pressure perturbs an equilibrium because the reaction quotient is shifted away from the equilibrium value. Changing the temperature of a system at equilibrium has a different effect: A change in temperature actually changes the value of the equilibrium constant. However, we can qualitatively predict the effect of the temperature change by treating it as a stress on the system and applying Le Chatelier's principle.

When hydrogen reacts with gaseous iodine, heat is evolved.

$$\mathrm{H_2}\,(g) + \mathrm{I_2}\,(g) \rightleftharpoons 2\,\mathrm{HI}\,(g) \quad \Delta H = -9.4\ \mathrm{kJ\ (exothermic)} \tag{7.3.5}$$

Because this reaction is exothermic, we can write it with heat as a product.

$$\mathrm{H_2}\,(g) + \mathrm{I_2}\,(g) \rightleftharpoons 2\,\mathrm{HI}\,(g) + \mathrm{heat} \tag{7.3.6}$$

Increasing the temperature of the reaction increases the internal energy of the system. Thus, increasing the temperature has the effect of increasing the amount of one of the products of this reaction. The reaction shifts to the left to relieve the stress, and there is an increase in the concentration of H_2 and I_2 and a reduction in the concentration of HI. Lowering the temperature of this system reduces the amount of energy present, favors the production of heat, and favors the formation of hydrogen iodide.

When we change the temperature of a system at equilibrium, the equilibrium constant for the reaction changes. Lowering the temperature in the HI system increases the equilibrium constant: At the new equilibrium the concentration of HI has increased and

the concentrations of H_2 and I_2 decreased. Raising the temperature decreases the value of the equilibrium constant, from 67.5 at 357 °C to 50.0 at 400 °C.

Temperature affects the equilibrium between $\mathbf{NO_2}$ and $\mathbf{N_2O_4}$ in this reaction

$$\mathbf{N_2O_4\,(g)} \rightleftharpoons \mathbf{2\,NO_2\,(g)} \quad \Delta H = 57.20\ \mathbf{kJ} \tag{7.3.7}$$

The positive ΔH value tells us that the reaction is endothermic and could be written

$$\mathbf{heat + N_2O_4\,(g)} \rightleftharpoons \mathbf{2\,NO_2\,(g)} \tag{7.3.8}$$

At higher temperatures, the gas mixture has a deep brown color, indicative of a significant amount of brown $\mathbf{NO_2}$ molecules. If, however, we put a stress on the system by cooling the mixture (withdrawing energy), the equilibrium shifts to the left to supply some of the energy lost by cooling. The concentration of colorless $\mathbf{N_2O_4}$ increases, and the concentration of brown $\mathbf{NO_2}$ decreases, causing the brown color to fade.

The overview of how different disturbances affect the reaction equilibrium properties is tabulated in Table **7.3.1**.

Table **7.3.1**: Effects of Disturbances of Equilibrium and K

Disturbance	Observed Change as Equilibrium is Restored	Direction of Shift	Effect on K
reactant added	added reactant is partially consumed	toward products	none
product added	added product is partially consumed	toward reactants	none
decrease in volume/increase in gas pressure	pressure decreases	toward side with fewer moles of gas	none
increase in volume/decrease in gas pressure	pressure increases	toward side with more moles of gas	none
temperature increase	heat is absorbed	toward products for endothermic, toward reactants for exothermic	changes
temperature decrease	heat is given off	toward reactants for endothermic, toward products for exothermic	changes

Example 7.3.1

Write an equilibrium constant expression for each reaction and use this expression to predict what will happen to the concentration of the substance in bold when the indicated change is made if the system is to maintain equilibrium.

a. $\mathbf{2}HgO_{(s)} \rightleftharpoons \mathbf{2}Hg_{(l)} + \mathbf{O_{2(g)}}$: the amount of HgO is doubled.
b. $NH_4HS_{(s)} \rightleftharpoons \mathbf{NH_{3(g)}} + H_2S_{(g)}$: the concentration of H_2S is tripled.
c. $\mathbf{n\text{-}butane}_{(g)} \rightleftharpoons isobutane_{(g)}$: the concentration of isobutane is halved.

Given: equilibrium systems and changes

Asked for: equilibrium constant expressions and effects of changes

Strategy:

Write the equilibrium constant expression, remembering that pure liquids and solids do not appear in the expression. From this expression, predict the change that must occur to maintain equilibrium when the indicated changes are made.

Solution:

Because $HgO_{(s)}$ and $Hg_{(l)}$ are pure substances, they do not appear in the equilibrium constant expression. Thus, for this reaction, $K = [O_2]$. The equilibrium concentration of O_2 is a constant and does not depend on the amount of HgO present. Hence adding more HgO will not affect the equilibrium concentration of O_2, so no compensatory change is necessary.

NH_4HS does not appear in the equilibrium constant expression because it is a solid. Thus $K = [NH_3][H_2S]$, which means that the concentrations of the products are inversely proportional. If adding H_2S triples the H_2S concentration, for example, then the NH_3 concentration must decrease by about a factor of 3 for the system to remain at equilibrium so that the product of the concentrations equals K.

For this reaction, $K = \frac{[isobutane]}{[n\text{-}butane]}$, so halving the concentration of isobutane means that the n-butane concentration must also decrease by about half if the system is to maintain equilibrium.

? Exercise 7.3.1

Write an equilibrium constant expression for each reaction. What must happen to the concentration of the substance in bold when the indicated change occurs if the system is to maintain equilibrium?

a. $\mathbf{HBr}(g) + NaH(s) \rightleftharpoons NaBr(s) + \mathbf{H_2}(g)$: the concentration of **HBr** is decreased by a factor of 3.
b. $6\,Li(s) + \mathbf{N_2}(g) \rightleftharpoons 2\,Li_3N(s)$: the amount of **Li** is tripled.
c. $\mathbf{SO_2}(g) + Cl_2(g) \rightleftharpoons SO_2Cl_2(l)$: the concentration of $\mathbf{Cl_2}$ is doubled.

Answer a

$K = \frac{[H_2]}{[HBr]}$; $[H_2]$ must decrease by about a factor of 3.

Answer b

$K = \frac{1}{[N_2]}$; solid lithium does not appear in the equilibrium constant expression, so no compensatory change is necessary.

Answer c

$K = \frac{1}{[SO_2][Cl_2]}$; $[SO_2]$ must decrease by about half.



Le Chatelier's Principle (Changes in Temperature):

Le Chatelier's Principle (Changes in Temperature)(opens in new window) [youtu.be]

Catalysts Do Not Affect Equilibrium

As we learned during our study of kinetics, a catalyst can speed up the rate of a reaction. Though this increase in reaction rate may cause a system to reach equilibrium more quickly (by speeding up the forward and reverse reactions), a catalyst has no effect on the value of an equilibrium constant nor on equilibrium concentrations. The interplay of changes in concentration or pressure,

temperature, and the lack of an influence of a catalyst on a chemical equilibrium is illustrated in the industrial synthesis of ammonia from nitrogen and hydrogen according to the equation

$$\mathrm{N_2(g) + 3\,H_2(g) \rightleftharpoons 2\,NH_3(g)} \tag{7.3.9}$$

A large quantity of ammonia is manufactured by this reaction. Each year, ammonia is among the top 10 chemicals, by mass, manufactured in the world. About 2 billion pounds are manufactured in the United States each year. Ammonia plays a vital role in our global economy. It is used in the production of fertilizers and is, itself, an important fertilizer for the growth of corn, cotton, and other crops. Large quantities of ammonia are converted to nitric acid, which plays an important role in the production of fertilizers, explosives, plastics, dyes, and fibers, and is also used in the steel industry.

Fritz Haber

Haber was born in Breslau, Prussia (presently Wroclaw, Poland) in December 1868. He went on to study chemistry and, while at the University of Karlsruhe, he developed what would later be known as the Haber process: the catalytic formation of ammonia from hydrogen and atmospheric nitrogen under high temperatures and pressures. For this work, Haber was awarded the 1918 Nobel Prize in Chemistry for synthesis of ammonia from its elements (Equation 7.3.9). The Haber process was a boon to agriculture, as it allowed the production of fertilizers to no longer be dependent on mined feed stocks such as sodium nitrate.



Figure **7.3.1**: The work of Nobel Prize recipient Fritz Haber revolutionized agricultural practices in the early 20th century. His work also affected wartime strategies, adding chemical weapons to the artillery.

Currently, the annual production of synthetic nitrogen fertilizers exceeds 100 million tons and synthetic fertilizer production has increased the number of humans that arable land can support from 1.9 persons per hectare in 1908 to 4.3 in 2008. The availability of nitrogen is a strong limiting factor to the growth of plants. Despite accounting for 78% of air, diatomic nitrogen ($\mathrm{N_2}$) is nutritionally unavailable to a majority of plants due the tremendous stability of the nitrogen-nitrogen triple bond. Therefore, the nitrogen must be converted to a more bioavailable form (this conversion is called nitrogen fixation). Legumes achieve this conversion at ambient temperature by exploiting bacteria equipped with suitable enzymes.

In addition to his work in ammonia production, Haber is also remembered by history as one of the fathers of chemical warfare. During World War I, he played a major role in the development of poisonous gases used for trench warfare. Regarding his role in these developments, Haber said, “During peace time a scientist belongs to the World, but during war time he belongs to his country.”[1] Haber defended the use of gas warfare against accusations that it was inhumane, saying that death was death, by whatever means it was inflicted. He stands as an example of the ethical dilemmas that face scientists in times of war and the double-edged nature of the sword of science.

Like Haber, the products made from ammonia can be multifaceted. In addition to their value for agriculture, nitrogen compounds can also be used to achieve destructive ends. Ammonium nitrate has also been used in explosives, including improvised explosive devices. Ammonium nitrate was one of the components of the bomb used in the attack on the Alfred P. Murrah Federal Building in downtown Oklahoma City on April 19, 1995.

Summary

Systems at equilibrium can be disturbed by changes to temperature, concentration, and, in some cases, volume and pressure; volume and pressure changes will disturb equilibrium if the number of moles of gas is different on the reactant and product sides of the reaction. The system's response to these disturbances is described by Le Chatelier's principle: The system will respond in a way that counteracts the disturbance. Not all changes to the system result in a disturbance of the equilibrium. Adding a catalyst affects

the rates of the reactions but does not alter the equilibrium, and changing pressure or volume will not significantly disturb systems with no gases or with equal numbers of moles of gas on the reactant and product side.

Footnotes

1. 1 Herrlich, P. “The Responsibility of the Scientist: What Can History Teach Us About How Scientists Should Handle Research That Has the Potential to Create Harm?” *EMBO Reports* 14 (2013): 759–764.

Glossary

Le Chatelier's principle

when a chemical system at equilibrium is disturbed, it returns to equilibrium by counteracting the disturbance

position of equilibrium

concentrations or partial pressures of components of a reaction at equilibrium (commonly used to describe conditions before a disturbance)

stress

change to a reaction's conditions that may cause a shift in the equilibrium

Contributors and Attributions

- Paul Flowers (University of North Carolina - Pembroke), Klaus Theopold (University of Delaware) and Richard Langley (Stephen F. Austin State University) with contributing authors. Textbook content produced by OpenStax College is licensed under a Creative Commons Attribution License 4.0 license. Download for free at http://cnx.org/contents/85abf193-2bd...a7ac8df6@9.110).

7.3: Chemical Equilibrium is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

- **15.7: Le Chatelier's Principle** is licensed CC BY-NC-SA 3.0.

7.4: Catalysis

Learning Objectives

By the end of this section, you will be able to:

- Explain the function of a catalyst in terms of reaction mechanisms and potential energy diagrams
- List examples of catalysis in natural and industrial processes

Among the factors affecting chemical reaction rates discussed earlier in this chapter was the presence of a *catalyst*, a substance that can increase the reaction rate without being consumed in the reaction. The concepts introduced in the previous section on reaction mechanisms provide the basis for understanding how catalysts are able to accomplish this very important function.

Figure **7.4.1** shows reaction diagrams for a chemical process in the absence and presence of a catalyst. Inspection of the diagrams reveals several traits of these reactions. Consistent with the fact that the two diagrams represent the same overall reaction, both curves begin and end at the same energies (in this case, because products are more energetic than reactants, the reaction is endothermic). The reaction mechanisms, however, are clearly different. The uncatalyzed reaction proceeds via a one-step mechanism (one transition state observed), whereas the catalyzed reaction follows a two-step mechanism (two transition states observed) with *a notably lesser activation energy*. This difference illustrates the means by which a catalyst functions to accelerate reactions, namely, by providing an alternative reaction mechanism with a lower activation energy. Although the catalyzed reaction mechanism for a reaction needn't necessarily involve a different number of steps than the uncatalyzed mechanism, it must provide a reaction path whose rate determining step is faster (lower E_a).

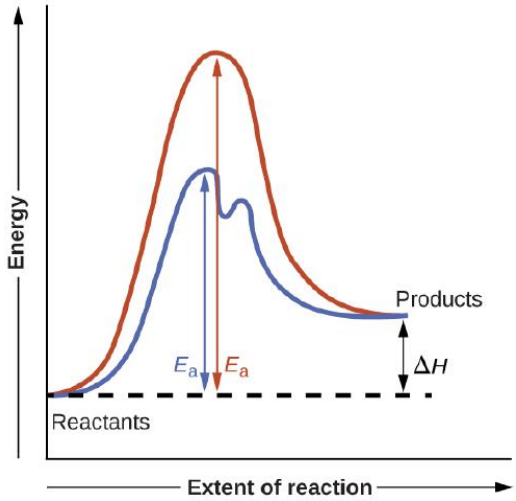
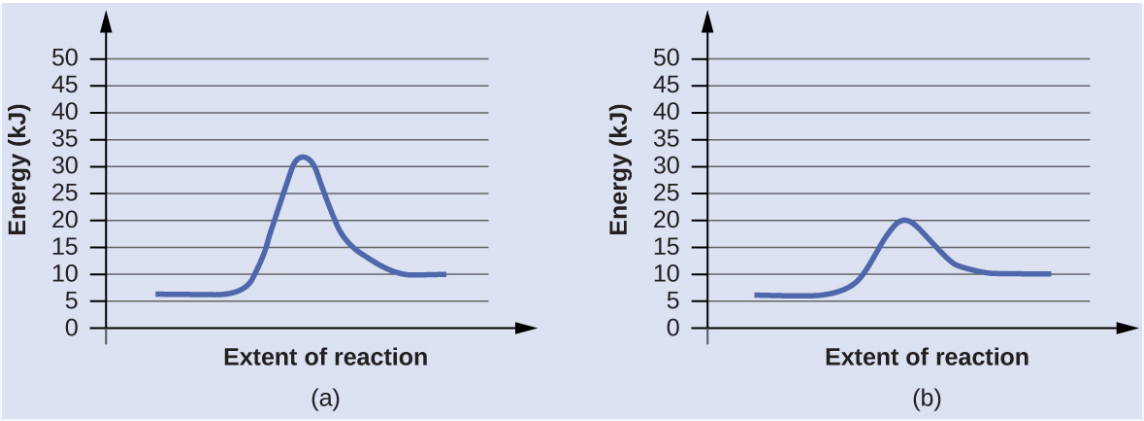


Figure **7.4.1**: Reaction diagrams for an endothermic process in the absence (red curve) and presence (blue curve) of a catalyst. The catalyzed pathway involves a two-step mechanism (note the presence of two transition states) and an intermediate species (represented by the valley between the two transitions states).

Example 7.4.1: Reaction Diagrams for Catalyzed Reactions

The two reaction diagrams here represent the same reaction: one without a catalyst and one with a catalyst. Estimate the activation energy for each process, and identify which one involves a catalyst.



Solution

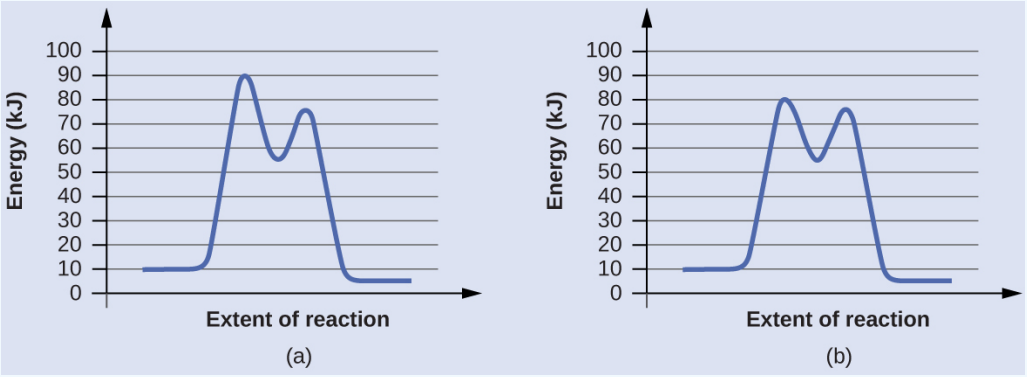
Activation energies are calculated by subtracting the reactant energy from the transition state energy.

$$\text{diagram}(a): E_a = 32kJ - 6kJ = 26kJ$$
$$\text{diagram}(b): E_a = 20kJ - 6kJ = 14kJ$$

The catalyzed reaction is the one with lesser activation energy, in this case represented by diagram b.

? Exercise 7.4.1

Reaction diagrams for a chemical process with and without a catalyst are shown below. Both reactions involve a two-step mechanism with a rate-determining first step. Compute activation energies for the first step of each mechanism, and identify which corresponds to the catalyzed reaction. How do the second steps of these two mechanisms compare?



Answer

For the first step, E_a = 80 kJ for (a) and 70 kJ for (b), so diagram (b) depicts the catalyzed reaction. Activation energies for the second steps of both mechanisms are the same, 20 kJ.

7.4.1: Homogeneous Catalysts

A homogeneous catalyst is present in the same phase as the reactants. It interacts with a reactant to form an intermediate substance, which then decomposes or reacts with another reactant in one or more steps to regenerate the original catalyst and form product.

As an important illustration of homogeneous catalysis, consider the earth's ozone layer. Ozone in the upper atmosphere, which protects the earth from ultraviolet radiation, is formed when oxygen molecules absorb ultraviolet light and undergo the reaction:

$$3O_2(g) \xrightarrow{h\nu} 2O_3(g)$$

Ozone is a relatively unstable molecule that decomposes to yield diatomic oxygen by the reverse of this equation. This decomposition reaction is consistent with the following two-step mechanism:

$$O_3 \longrightarrow O_2 + O$$
$$O + O_3 \longrightarrow 2O_2$$

A number of substances can catalyze the decomposition of ozone. For example, the nitric oxide–catalyzed decomposition of ozone is believed to occur via the following three-step mechanism:

$$NO(g) + O_3(g) \longrightarrow NO_2(g) + O_2(g)$$
$$O_3(g) \longrightarrow O_2(g) + O(g)$$
$$NO_2(g) + O(g) \longrightarrow NO(g) + O_2(g)$$

As required, the overall reaction is the same for both the two-step uncatalyzed mechanism and the three-step NO-catalyzed mechanism:

$$2O_3(g) \longrightarrow 3O_2(g)$$

Notice that NO is a reactant in the first step of the mechanism and a product in the last step. This is another characteristic trait of a catalyst: Though it participates in the chemical reaction, it is not consumed by the reaction.

Portrait of a Chemist: Mario J. Molina

The 1995 Nobel Prize in Chemistry was shared by Paul J. Crutzen, Mario J. Molina (Figure **7.4.2**), and F. Sherwood Rowland "for their work in atmospheric chemistry, particularly concerning the formation and decomposition of ozone."[1] Molina's initial discovery of stratospheric depletion of ozone by chlorine atoms was done at the University of California Irvine, he later moved to the NASA/Jet Propulsion Laboratory, MIT and the University of California, San Diego. At the time of his death in 2020 Molina, a Mexican citizen had established a new center for the study of energy and the environment in Mexico City.

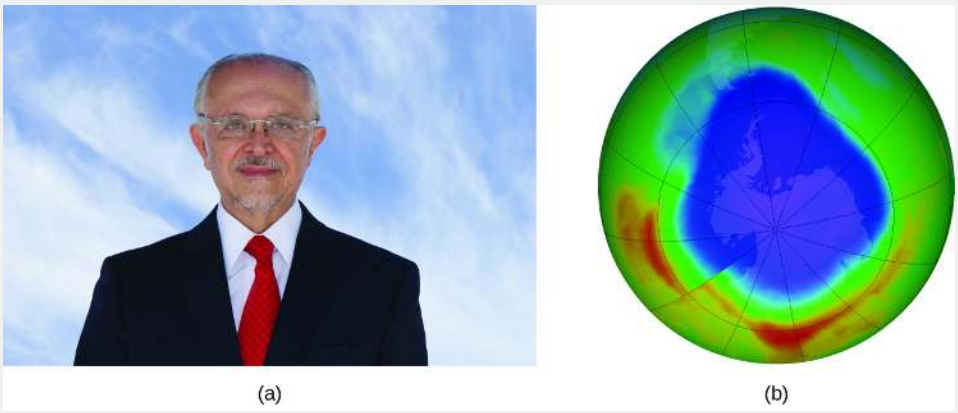


Figure **7.4.2**: (a) Mexican chemist Mario Molina (1943 –) shared the Nobel Prize in Chemistry in 1995 for his (b) early research on stratospheric depletion of ozone and later the Antarctic ozone hole. (credit a: courtesy of Mario Molina; credit b: modification of work by NASA)

In 1974, Molina and Rowland published a paper in the journal *Nature* detailing the threat of chlorofluorocarbon gases to the stability of the ozone layer in earth's upper atmosphere. The ozone layer protects earth from solar radiation by absorbing ultraviolet light. As chemical reactions deplete the amount of ozone in the upper atmosphere, a measurable "hole" forms above Antarctica, and an increase in the amount of solar ultraviolet radiation— strongly linked to the prevalence of skin cancers—reaches earth's surface. The work of Molina and Rowland was instrumental in the adoption of the Montreal Protocol, an international treaty signed in 1987 that successfully began phasing out production of chemicals linked to ozone destruction.

Molina and Rowland demonstrated that chlorine atoms from human-made chemicals can catalyze ozone destruction in a process similar to that by which NO accelerates the depletion of ozone. Chlorine atoms are generated when chlorocarbons or chlorofluorocarbons—once widely used as refrigerants and propellants—are photochemically decomposed by ultraviolet light or react with hydroxyl radicals. A sample mechanism is shown here using methyl chloride:

$$CH_3Cl + OH \longrightarrow Cl + \text{ other products} \tag{7.4.1}$$

Chlorine radicals break down ozone and are regenerated by the following catalytic cycle:

$$Cl + O_3 \longrightarrow ClO + O_2$$
$$ClO + O \longrightarrow Cl + O_2$$

overall Reaction: $O_3 + O \longrightarrow 2O_2$ \nonumber \]

A single monatomic chlorine can break down thousands of ozone molecules. Luckily, the majority of atmospheric chlorine exists as the catalytically inactive forms Cl_2 and $ClONO_2$.

Enzymes in the human body act as catalysts for important chemical reactions in cellular metabolism. As such, a deficiency of a particular enzyme can translate to a life-threatening disease. G6PD (glucose-6-phosphate dehydrogenase) deficiency, a genetic condition that results in a shortage of the enzyme glucose-6-phosphate dehydrogenase, is the most common enzyme deficiency in humans. This enzyme, shown in Figure 12.21, is the rate-limiting enzyme for the metabolic pathway that supplies NADPH to cells (Figure **7.4.4**).

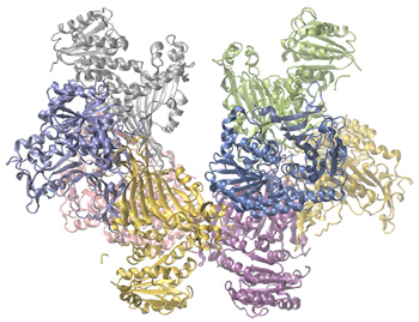


Figure 12.21 Glucose-6-phosphate dehydrogenase is a rate-limiting enzyme for the metabolic pathway that supplies NADPH to cells.

A disruption in this pathway can lead to reduced glutathione in red blood cells; once all glutathione is consumed, enzymes and other proteins such as hemoglobin are susceptible to damage. For example, hemoglobin can be metabolized to bilirubin, which leads to jaundice, a condition that can become severe. People who suffer from G6PD deficiency must avoid certain foods and medicines containing chemicals that can trigger damage their glutathione-deficient red blood cells.

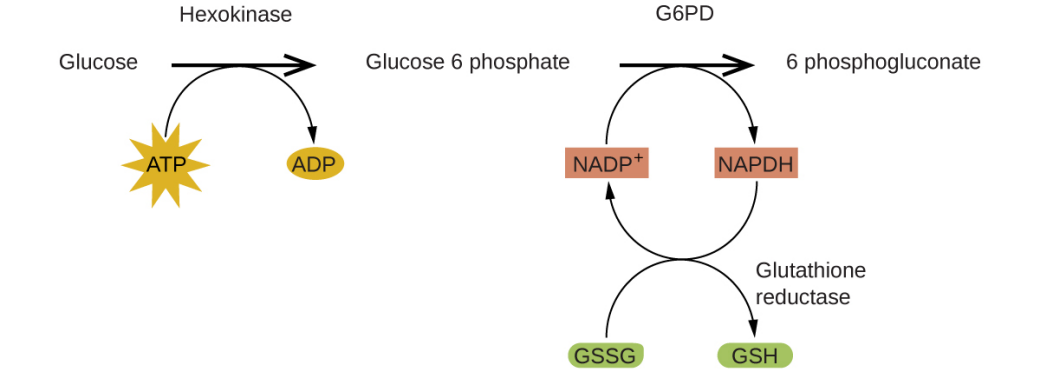


Figure **7.4.4**: In the mechanism for the pentose phosphate pathway, G6PD catalyzes the reaction that regulates NADPH, a co-enzyme that regulates glutathione, an antioxidant that protects red blood cells and other cells from oxidative damage.

7.4.2: Heterogeneous Catalysts

A heterogeneous catalyst is a catalyst that is present in a different phase (usually a solid) than the reactants. Such catalysts generally function by furnishing an active surface upon which a reaction can occur. Gas and liquid phase reactions catalyzed by heterogeneous catalysts occur on the surface of the catalyst rather than within the gas or liquid phase.

Heterogeneous catalysis typically involves the following processes:

1. Adsorption of the reactant(s) onto the surface of the catalyst
2. Activation of the adsorbed reactant(s)
3. Reaction of the adsorbed reactant(s)

Figure **7.4.5**: illustrates the steps of a mechanism for the reaction of compounds containing a carbon–carbon double bond with hydrogen on a nickel catalyst. Nickel is the catalyst used in the hydrogenation of polyunsaturated fats and oils (which contain several carbon–carbon double bonds) to produce saturated fats and oils (which contain only carbon–carbon single bonds).

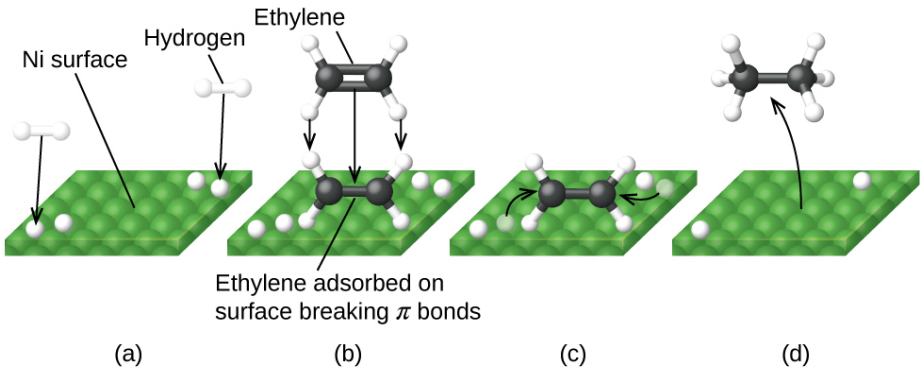


Figure **7.4.5**: Mechanism for the Ni-catalyzed reaction $C_2H_4 + H_2 \longrightarrow C_2H_6$. (a) Hydrogen is adsorbed on the surface, breaking the H–H bonds and forming Ni–H bonds. (b) Ethylene is adsorbed on the surface, breaking the C–C π-bond and forming Ni–C bonds. (c) Atoms diffuse across the surface and form new C–H bonds when they collide. (d) C_2H_6 molecules desorb from the Ni surface.

Many important chemical products are prepared via industrial processes that use heterogeneous catalysts, including ammonia, nitric acid, sulfuric acid, and methanol. Heterogeneous catalysts are also used in the catalytic converters found on most gasoline-powered automobiles (Figure **7.4.6**).

Chemistry in Everyday Life: Automobile Catalytic Converters

Scientists developed catalytic converters to reduce the amount of toxic emissions produced by burning gasoline in internal combustion engines. By utilizing a carefully selected blend of catalytically active metals, it is possible to effect complete combustion of all carbon-containing compounds to carbon dioxide while also reducing the output of nitrogen oxides. This is particularly impressive when we consider that one step involves adding more oxygen to the molecule and the other involves removing the oxygen (Figure **7.4.6**).

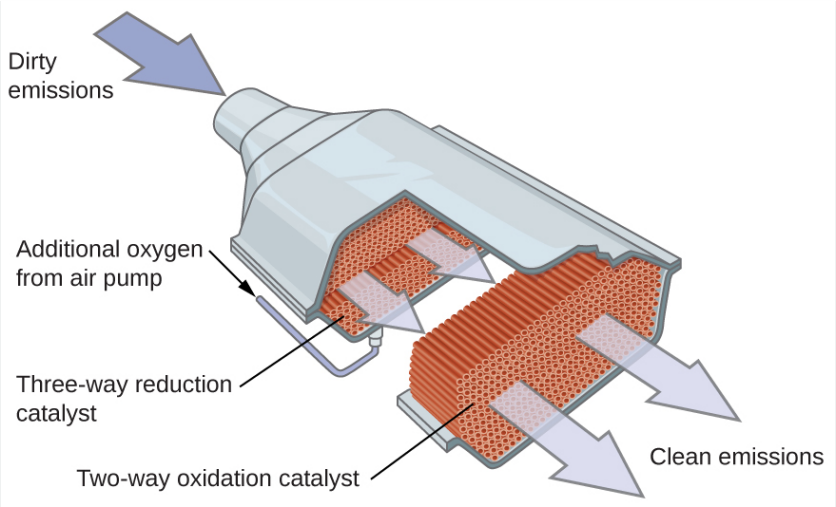


Figure **7.4.6**: A catalytic converter allows for the combustion of all carbon-containing compounds to carbon dioxide, while at the same time reducing the output of nitrogen oxide and other pollutants in emissions from gasoline-burning engines.

Most modern, three-way catalytic converters possess a surface impregnated with a platinum-rhodium catalyst, which catalyzes the conversion of nitric oxide into dinitrogen and oxygen as well as the conversion of carbon monoxide and hydrocarbons such as octane into carbon dioxide and water vapor:

$$2NO_2(g) \longrightarrow N_2(g) + 2O_2(g)$$
$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$
$$2C_8H_{18}(g) + 25O_2(g) \longrightarrow 16CO_2(g) + 18H_2O(g)$$

In order to be as efficient as possible, most catalytic converters are preheated by an electric heater. This ensures that the metals in the catalyst are fully active even before the automobile exhaust is hot enough to maintain appropriate reaction temperatures.

Link to Learning

The LibreTexts provides a thorough explanation of how catalytic converters work.

How Sciences Interconnect: Enzyme Structure and Function

The study of enzymes is an important interconnection between biology and chemistry. Enzymes are usually proteins (polypeptides) that help to control the rate of chemical reactions between biologically important compounds, particularly those that are involved in cellular metabolism. Different classes of enzymes perform a variety of functions, as shown in Table **7.4.1**.

Table **7.4.1**: Classes of Enzymes and Their Functions

Class	Function
oxidoreductases	redox reactions
transferases	transfer of functional groups
hydrolases	hydrolysis reactions
lyases	group elimination to form double bonds
isomerases	isomerization
ligases	bond formation with ATP hydrolysis

Enzyme molecules possess an active site, a part of the molecule with a shape that allows it to bond to a specific substrate (a reactant molecule), forming an enzyme-substrate complex as a reaction intermediate. There are two models that attempt to explain

how this active site works. The most simplistic model is referred to as the lock-and-key hypothesis, which suggests that the molecular shapes of the active site and substrate are complementary, fitting together like a key in a lock. The induced fit hypothesis, on the other hand, suggests that the enzyme molecule is flexible and changes shape to accommodate a bond with the substrate. This is not to suggest that an enzyme's active site is completely malleable, however. Both the lock-and-key model and the induced fit model account for the fact that enzymes can only bind with specific substrates, since in general a particular enzyme only catalyzes a particular reaction (Figure **7.4.7**).

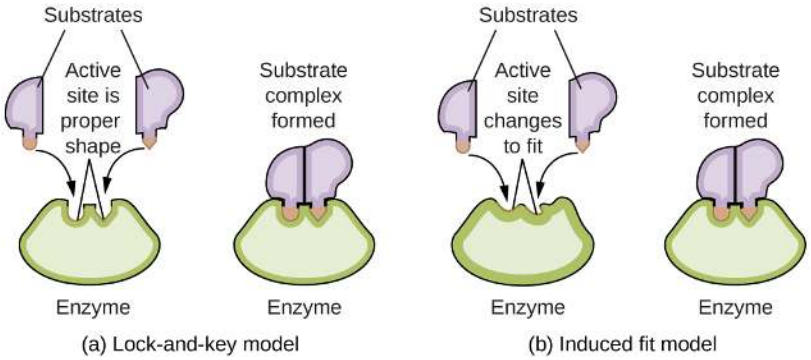


Figure **7.4.7**: (a) According to the lock-and-key model, the shape of an enzyme's active site is a perfect fit for the substrate. (b) According to the induced fit model, the active site is somewhat flexible, and can change shape in order to bond with the substrate.

Link to Learning

The Royal Society of Chemistry provides an excellent introduction to enzymes for students and teachers.

7.4.3: Footnotes

- 1"The Nobel Prize in Chemistry 1995," Nobel Prize.org, accessed February 18, 2015, http://www.nobelprize.org/nobel_priz...aureates/1995/.

This page titled 7.4: Catalysis is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **12.7: Catalysis** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

7.5: Case Study- Balancing Acts in Pharmacological Synthesis

Introduction: Chemical equations are the language through which chemists communicate the subtleties of chemical reactions. Balancing these equations is crucial in pharmacological research, where the synthesis of new drug molecules is both an art and a science. This case study explores the importance of balancing chemical equations in synthesizing new drugs and how this relates to enzyme kinetics in the body.

Scenario: In Apex Pharmaceuticals' high-tech research laboratory, a team of researchers, including Dr. Sophie Lee, is on the verge of a breakthrough. They have developed a promising new drug molecule that could potentially treat a rare genetic disorder. However, before they can move forward with production and trials, they must first balance the chemical equation for the drug's synthesis reaction to ensure the process is efficient, cost-effective, and yields the correct product in the desired quantities.

The Art of Balancing Equations: Dr. Lee and her team meticulously account for each atom of the reactants and products, adhering to the law of conservation of mass. They adjust coefficients to balance the number of atoms on both sides of the equation, a step critical for the synthesis process to proceed correctly and safely.

Case Study Questions:

1. **Why is balancing chemical equations important in drug synthesis?**
2. **How do reaction rates relate to enzyme kinetics?**

Hands-On Classroom Activities:

1. **Synthesis Lab:** In the "Synthesis Lab" activity, students will synthesize aspirin and are required to balance the chemical equation for this reaction. This exercise is designed to connect their understanding of chemical reactions and stoichiometry with the practical aspects of drug synthesis and pharmaceutical chemistry.
2. **Enzyme Kinetics Experiment:** During the Enzyme Kinetics Experiment, students will investigate reaction rates by observing enzyme-catalyzed reactions. They will then relate their observations to the principles of balancing chemical equations, thereby enhancing their understanding of the role of enzymes in biological reactions and the importance of precise chemical equations in biochemistry.

Conclusion: For Dr. Lee and her team at Apex Pharmaceuticals, balancing chemical equations is not just a necessary step in synthesizing new drug molecules—it is a critical process that affects every stage from design to delivery. It ensures that each synthesis step is predictable and controllable, which is vital for the safe and effective production of pharmaceuticals. Moreover, by understanding the principles of enzyme kinetics and reaction rates, researchers can better anticipate how a drug will perform in vivo, ultimately leading to more effective treatments with fewer side effects. The meticulous balancing of chemical equations thus stands as the cornerstone of successful drug development and patient care.

7.5: Case Study- Balancing Acts in Pharmacological Synthesis is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

7.E: Exercises

Multiple choice

1. Select the correct set of coefficients for the **balanced** chemical equation:

   ____$C_6H_{10}(l)$ + ____$O_2(g)$ → ____$CO_2(g)$ + ____$H_2O(g)$

   a. 1, 9, 6, 5

   b. 1, 18, 12, 10

   c. 2, 17, 6, 5

   d. 2, 17, 12, 10

2. Select the correct set of coefficients for the **balanced** chemical equation:

   ____$NH_3(g)$ + ____$CuO(s)$ → ____$N_2(g)$ + ____$Cu(s)$ + ____$H_2O(l)$

   a. 2, 3, 1, 3, 3

   b. 3, 2, 3, 2, 2

   c. 2, 3, 1, 3, 2

   d. 2, 4, 2, 4, 4

3. Which of the following chemical equations is the correct, balanced molecular equation for the reaction of solid aluminum hydroxide with aqueous sulfuric acid to obtain aqueous aluminum sulfate and water?

   a. $2AlOH(s) + H_2SO_4(aq) \rightarrow Al_2SO_4(aq) + 2H_2O(l)$

   b. $Al(OH)_2(s) + H_2SO_4(aq) \rightarrow AlSO_4(aq) + 2H_2O(l)$

   c. $2Al(OH)_3(s) + 3H_2SO_4(aq) \rightarrow Al_2(SO_4)_3(aq) + 6H_2O(l)$

   d. $Al(OH)_3(s) + 3HSO_4(aq) \rightarrow Al(SO_4)_3(aq) + 3H_2O(l)$

4. Which of the following chemical equations is the correct, balanced molecular equation for the reaction of aqueous sodium phosphate with aqueous silver nitrate to yield solid silver phosphate and aqueous sodium nitrate?

   a. $NaPO_4(aq) + AgNO_3(aq) \rightarrow AgPO_4(s) + NaNO_3(aq)$

   b. $Na_3PO_4(aq) + AgNO_3(aq) \rightarrow AgPO_4(s) + Na_3NO_3(aq)$

   c. $Na_2PO_4(aq) + 2AgNO_3(aq) \rightarrow Ag_2PO_4(s) + 2NaNO_3(aq)$

   d. $Na_3PO_4(aq) + 3AgNO_3(aq) \rightarrow Ag_3PO_4(s) + 3NaNO_3(aq)$

5. Choose the words that will correctly complete the following sentence: Heat is the transfer of _____ energy between two bodies at different _____.

   a. potential, positions

   b. potential, temperatures

   c. thermal, positions

   d. thermal, temperatures

6. Select the correct choice for the following reaction: $H_2(g) \rightarrow 2H(g)$.

   a. This reaction requires energy and represents an endothermic process.

   b. This reaction releases energy and represents an exothermic process.

   c. This reaction requires energy and represents an exothermic process.

   d. This reaction releases energy and represents an endothermic process.

7. Which of the following stresses would cause the equilibrium concentration of SO_3 to **decrease** for the following reaction:

$O_2(g) + NO_2(g) \rightleftharpoons NO(g) + SO_3(g)$?

a. Adding SO_2

b. Removing NO_2

c. Removing NO

d. All of the above

8. Which of the following stresses would cause the equilibrium concentration of SO_2Cl_2 to **increase** for the following **endothermic** reaction:

$SO_2Cl_2(g) \rightleftharpoons SO_2(g) + Cl_2(g)$

a. Increasing the temperature

b. Removing SO_2

c. Adding Cl_2

d. None of the above

9. Which of the following statements regarding a catalyst is **true**?

a. A catalyst is consumed in a chemical reaction.

b. A catalyst increases the thermal energy of the reactants.

c. A catalyst increases the stability of the product.

d. A catalyst lowers the activation energy for a reaction.

10. Nitrogen and oxygen react at high temperatures to form nitrogen monoxide. What will happen to the concentrations of N_2, O_2, and NO at equilibrium if a catalyst is added?

a. The equilibrium concentrations will increase.

b. The equilibrium concentrations will not change.

c. The equilibrium concentrations will decrease.

d. The N_2 and O_2 concentrations will decrease while the NO concentration will increase.

Easy

1. Balance the following equations:

a. $PCl_5(s) + H_2O(l) \rightarrow POCl_3(l) + HCl(aq)$

b. $Cu(s) + HNO_3(aq) \rightarrow Cu(NO_3)_2(aq) + H_2O(l) + NO_2(g)$

2. Balance the following equations:

a. $H_2(g) + I_2(s) \rightarrow HI(s)$

b. $Fe(s) + O_2(g) \rightarrow Fe_2O_3(s)$

3. Balance the following equations:

a. $Na(s) + H_2O(l) \rightarrow NaOH(aq) + H_2(g)$

b. $(NH_4)_2Cr_2O_7(s) \rightarrow Cr_2O_3(s) + N_2(g) + H_2O(g)$

4. Balance the following equations:

a. $P_4(s) + Cl_2(g) \rightarrow PCl_3(l)$

b. $PtCl_4(s) \rightarrow Pt(s) + Cl_2(g)$

5. Balance the following equations:
   a. $Ag(s) + H_2S(g) + O_2(g) \rightarrow Ag_2S(s) + H_2O(l)$
   b. $P_4(s) + O_2(g) \rightarrow P_4O_{10}(s)$
6. Balance the following equations:
   a. $Pb(s) + H_2O(l) + O_2(g) \rightarrow Pb(OH)_2(s)$
   b. $Fe(s) + H_2O(l) \rightarrow Fe_3O_4(s) + H_2(g)$
7. Balance the following equations:
   a. $Sc_2O_3(s) + SO_3(g) \rightarrow Sc_2(SO_4)_3(s)$
   b. $Ca_3(PO_4)_2(aq) + H_3PO_4(aq) \rightarrow Ca(H_2PO_4)_2(aq)$
8. Balance the following equations:
   a. $Al(s) + H_2SO_4(aq) \rightarrow Al_2(SO_4)_3(aq) + H_2(g)$
   b. $TiCl_4(s) + H_2O(l) \rightarrow TiO_2(s) + HCl(aq)$
9. Suggest four ways in which the concentration of hydrazine (N_2H_4) could be increased in an equilibrium described by the following balanced endothermic reaction:

   $N_2(g) + 2H_2(g) \rightleftharpoons N_2H_4(g)$.
10. Suggest four ways in which the concentration of PH_3 could be increased in an equilibrium described by the following balanced endothermic reaction:

    $P_4(g) + 6H_2(g) \rightleftharpoons 4PH_3(g)$

Medium

1. Write a balanced molecular equation describing each of the following chemical reactions:
   a. Solid calcium carbonate is heated and decomposes to solid calcium oxide and carbon dioxide gas.
   b. Gaseous butane (C_4H_{10}) reacts with diatomic oxygen gas to yield gaseous carbon dioxide and water vapor
2. Write a balanced molecular equation describing each of the following chemical reactions:
   a. Aqueous solutions of magnesium chloride and sodium hydroxide react to produce solid magnesium hydroxide and aqueous sodium chloride
   b. Water vapor reacts with sodium metal to produce solid sodium hydroxide and hydrogen gas.
3. Write a balanced molecular equation describing each of the following chemical reactions:
   a. Solid potassium chlorate ($KClO_3$) decomposes to form solid potassium chloride and diatomic oxygen gas.
   b. Solid aluminum metal reacts with solid diatomic iodine to form solid Al_2I_6.
4. Write a balanced molecular equation describing each of the following chemical reactions:
   a. When solid sodium chloride is added to aqueous sulfuric acid, hydrogen chloride gas and aqueous sodium sulfate are produced.
   b. Aqueous solutions of phosphoric acid and potassium hydroxide react to produce aqueous potassium dihydrogen phosphate and liquid water.
5. Colorful fireworks often involved the decomposition of barium nitrate and potassium chlorate and the reaction of the metals magnesium, aluminum, and iron with oxygen.
   a. Write the formulas of barium nitrate and potassium chlorate.

b. The decomposition of solid potassium chlorate leads to the formation of solid potassium chloride and diatomic oxygen gas. Write a balanced equation for the reaction.

c. The decomposition of solid barium nitrate leads to the formation of solid barium oxide, diatomic nitrogen gas, and diatomic oxygen gas. Write a balanced equation for the reaction.

6. How will an increase in temperature affect each of the following equilibria? How will a decrease in the volume of the reaction vessel affect each?

a. $2NH_3(g) \rightleftharpoons N_2(g) + 3H_2(g)$ (endothermic)

b. $N_2(g) + O_2(g) \rightleftharpoons 2NO(g)$ (endothermic)

c. $2O_3(g) \rightleftharpoons 3O_2(g)$ (exothermic)

d. $CaO(s) + CO_2(g) \rightleftharpoons CaCO_3(s)$ (exothermic)

7. How will an increase in temperature affect each of the following equilibria? How will a decrease in the volume of the reaction vessel affect each?

a. $2H_2O(g) \rightleftharpoons 2H_2(g) + O_2(g)$ (endothermic)

b. $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$ (exothermic)

c. $2Br(g) \rightleftharpoons Br_2(g)$ (exothermic)

d. $H_2(g) + I_2(s) \rightleftharpoons 2HI(g)$ (endothermic)

8. Ammonia reacts with water according to this equation: $NH_3(aq) + H_2O(l) \rightleftharpoons NH_4^+(aq) + OH^-(aq)$. Will any of the following increase the percentage of ammonia that is converted to the ammonium ion in water?

a. Addition of NaOH

b. Addition of HCl

c. Addition of NH_4Cl

9. Acetic acid reacts with water according to this equation: $CH_3CO_2H(aq) + H_2O(l) \rightleftharpoons H_3O^+(aq) + CH_3CO_2^-(aq)$. Will any of the following increase the percentage of acetic acid that is converted to the acetate ion in water?

a. Addition of HCl

b. Addition of NaOH

c. Addition of $NaCH_3CO_2$

Challenge

1. A novel process for obtaining magnesium from seawater involves several reactions. Write a balanced chemical equation for each step of the process

a. The first step is decomposing solid calcium carbonate from seashells to form solid calcium oxide and gaseous carbon dioxide.

b. The second step is the formation of solid calcium hydroxide as the only product of the reaction of solid calcium oxide with liquid water.

c. Solid calcium hydroxide is added to the seawater, reacting with dissolved magnesium chloride to yield solid magnesium hydroxide and aqueous calcium chloride.

d. Solid magnesium hydroxide is added to a hydrochloric acid solution, producing dissolved magnesium chloride and liquid water.

e. Finally, the magnesium chloride is melted and electrolyzed to yield liquid magnesium metal and diatomic chlorine gas.

Health-Related Questions

1. The overall reaction that occurs in aerobic cellular respiration is the reaction between aqueous sucrose ($C_6H_{12}O_6$) and gaseous oxygen to produce gaseous carbon dioxide and water. Write a balanced chemical equation for this reaction.

2. Milk of magnesia (a suspension of solid magnesium hydroxide) is consumed (in some cases) due to excess stomach acid. Write a balanced chemical equation for the reaction of solid magnesium hydroxide with aqueous sulfuric acid to produce aqueous magnesium sulfate and water.

3. Alka-Seltzer tables contain solid sodium bicarbonate and citric acid ($H_3C_6H_5O_7$). When added to water, these solids react to produce gaseous carbon dioxide, aqueous sodium citrate (citrate has the formula $C_6H_5O_7^{3-}$), and water. Write a balanced chemical equation for the reaction of sodium bicarbonate with citric acid.

4. The following equilibrium reaction: $CO_2(g) + H_2O(l) \rightleftharpoons HCO_3^-(aq) + H^+(aq)$ is important in our bodies as it controls blood pH. Acidosis occurs when the concentration of H^+ in the bloodstream is too large. State three stresses (according to Le Châtelier's principle) that would lead to acidosis.

7.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

8: Gases, Liquids, and Solids

8.1: The Kinetic-Molecular Theory
8.2: Gas Pressure
8.3: The Gas Laws
8.4: Intermolecular Forces
8.5: Types of Solutions
8.6: Electrolytes
8.7: Concentration
8.7.1: Other Units for Solution Concentrations
8.8: Osmosis, Diffusion and Dialysis
8.9: Health Connections- Oxygen in the Body
8.10: Case Study- The Vital Breath – Kinetic Molecular Theory in Respiratory Care
8.E: Exercises

8: Gases, Liquids, and Solids is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

8.1: The Kinetic-Molecular Theory

Learning Objectives

- State the postulates of the kinetic-molecular theory
- Use this theory's postulates to explain the gas laws

The gas laws that we have seen to this point, as well as the ideal gas equation, are empirical, that is, they have been derived from experimental observations. The mathematical forms of these laws closely describe the macroscopic behavior of most gases at pressures less than about 1 or 2 atm. Although the gas laws describe relationships that have been verified by many experiments, they do not tell us why gases follow these relationships.

The **kinetic molecular theory** (KMT) is a simple microscopic model that effectively explains the gas laws described in previous modules of this chapter. This theory is based on the following five postulates described here. (Note: The term "molecule" will be used to refer to the individual chemical species that compose the gas, although some gases are composed of atomic species, for example, the noble gases.)

1. Gases are composed of molecules that are in continuous motion, travelling in straight lines and changing direction only when they collide with other molecules or with the walls of a container.
2. The molecules composing the gas are negligibly small compared to the distances between them.
3. The pressure exerted by a gas in a container results from collisions between the gas molecules and the container walls.
4. Gas molecules exert no attractive or repulsive forces on each other or the container walls; therefore, their collisions are *elastic* (do not involve a loss of energy).
5. The average kinetic energy of the gas molecules is proportional to the kelvin temperature of the gas.

The test of the KMT and its postulates is its ability to explain and describe the behavior of a gas. The various gas laws can be derived from the assumptions of the KMT, which have led chemists to believe that the assumptions of the theory accurately represent the properties of gas molecules. We will first look at the individual gas laws (Boyle's, Charles's, Amontons's, Avogadro's, and Dalton's laws) conceptually to see how the KMT explains them. Then, we will more carefully consider the relationships between molecular masses, speeds, and kinetic energies with temperature, and explain Graham's law.

8.1.1: The Kinetic-Molecular Theory Explains the Behavior of Gases, Part I

Recalling that gas pressure is exerted by rapidly moving gas molecules and depends directly on the number of molecules hitting a unit area of the wall per unit of time, we see that the KMT conceptually explains the behavior of a gas as follows:

- *Amontons's law.* If the temperature is increased, the average speed and kinetic energy of the gas molecules increase. If the volume is held constant, the increased speed of the gas molecules results in more frequent and more forceful collisions with the walls of the container, therefore increasing the pressure (Figure 8.1.1).
- *Charles's law.* If the temperature of a gas is increased, a constant pressure may be maintained only if the volume occupied by the gas increases. This will result in greater average distances traveled by the molecules to reach the container walls, as well as increased wall surface area. These conditions will decrease the both the frequency of molecule-wall collisions and the number of collisions per unit area, the combined effects of which balance the effect of increased collision forces due to the greater kinetic energy at the higher temperature.
- *Boyle's law.* If the gas volume volume of a given amount of gas at a given temperature is decreased (that is, if the gas is *compressed*), the molecules will be exposed to a decreased container wall area. Collisions with the container wall will therefore occur more frequently and the pressure exerted by the gas will increase (Figure 8.1.1).
- *Avogadro's law.* At constant pressure and temperature, the frequency and force of molecule-wall collisions are constant. Under such conditions, increasing the number of gaseous molecules will require a proportional increase in the container volume in order to yield a decrease in the number of collisions per unit area to compensate for the increased frequency of collisions (Figure 8.1.1).
- *Dalton's Law.* Because of the large distances between them, the molecules of one gas in a mixture bombard the container walls with the same frequency whether other gases are present or not, and the total pressure of a gas mixture equals the sum of the

(partial) pressures of the individual gases.

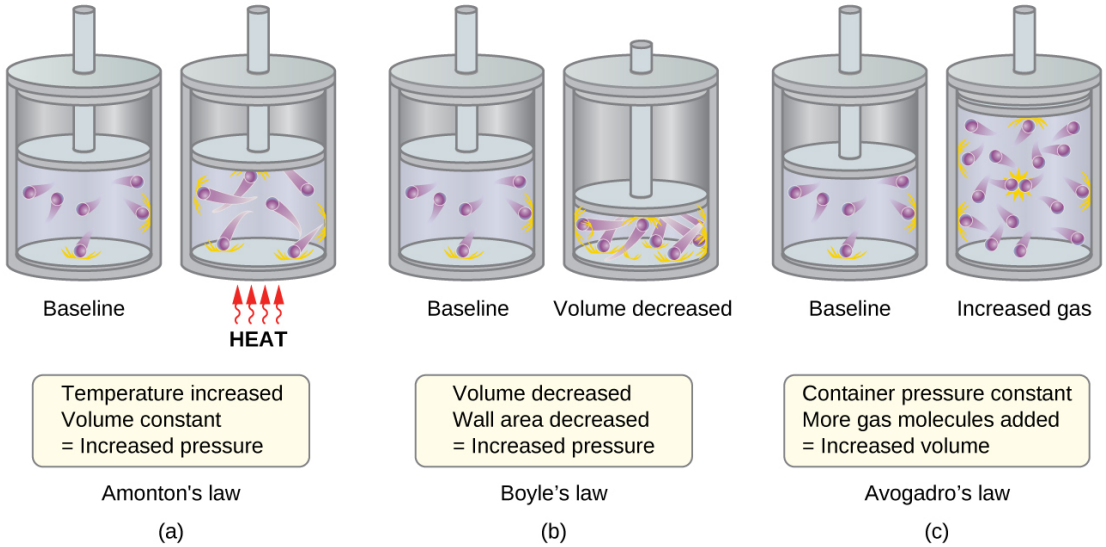


Figure 8.1.1: (a) When gas temperature increases, gas pressure increases due to increased force and frequency of molecular collisions. (b) When volume decreases, gas pressure increases due to increased frequency of molecular collisions. (c) When the amount of gas increases at a constant pressure, volume increases to yield a constant number of collisions per unit wall area per unit time.

8.1.2: molecular speeds and Kinetic Energy

The previous discussion showed that the KMT qualitatively explains the behaviors described by the various gas laws. The postulates of this theory may be applied in a more quantitative fashion to derive these individual laws. To do this, we must first look at speeds and kinetic energies of gas molecules, and the temperature of a gas sample.

In a gas sample, individual molecules have widely varying speeds; however, because of the *vast* number of molecules and collisions involved, the molecular speed distribution and average speed are constant. This molecular speed distribution is known as a Maxwell-Boltzmann distribution, and it depicts the relative numbers of molecules in a bulk sample of gas that possesses a given speed (Figure 8.1.2).

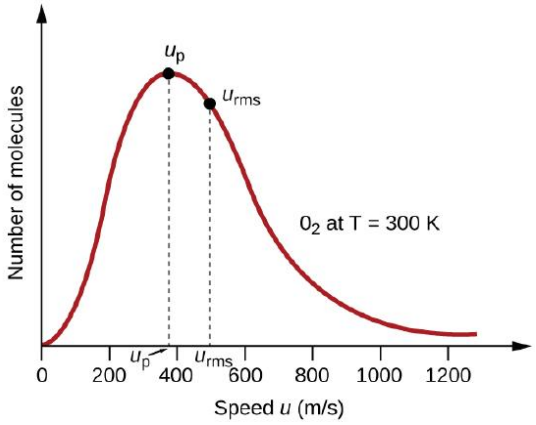


Figure 8.1.2: The molecular speed distribution for oxygen gas at 300 K is shown here. Very few molecules move at either very low or very high speeds. The number of molecules with intermediate speeds increases rapidly up to a maximum, which is the most probable speed, then drops off rapidly. Note that the most probable speed, v_p, is a little less than 400 m/s, while the root mean square speed, u_{rms}, is closer to 500 m/s.

The kinetic energy (KE) of a particle of mass (m) and speed (u) is given by:

$$KE = \frac{1}{2}mu^2$$

Expressing mass in kilograms and speed in meters per second will yield energy values in units of joules (J = kg m^2 s^{-2}). To deal with a large number of gas molecules, we use averages for both speed and kinetic energy. In the KMT, the root mean square speed of a particle, u_{rms}, is defined as the square root of the average of the squares of the speeds with n = the number of particles:

$$u_{rms} = \sqrt{\overline{u^2}} = \sqrt{\frac{u_1^2 + u_2^2 + u_3^2 + u_4^2 + \ldots}{n}}$$

The average kinetic energy for a mole of particles, KE_{avg}, is then equal to:

$$KE_{avg} = \frac{1}{2} M u_{rms}^2$$

where M is the molar mass expressed in units of kg/mol. The KE_{avg} of a mole of gas molecules is also directly proportional to the temperature of the gas and may be described by the equation:

$$KE_{avg} = \frac{3}{2} RT$$

where R is the gas constant and T is the kelvin temperature. When used in this equation, the appropriate form of the gas constant is 8.314 J/mol·K (8.314 kg $m^2 s^{-2} mol^{-1} K^{-1}$). These two separate equations for KE_{avg} may be combined and rearranged to yield a relation between molecular speed and temperature:

$$\frac{1}{2} M u_{rms}^2 = \frac{3}{2} RT$$

with

$$u_{rms} = \sqrt{\frac{3RT}{M}}$$

Example 8.1.1: Calculation of u_{rms}

Calculate the root-mean-square speed for a nitrogen molecule at 30 °C.

Solution

Convert the temperature into Kelvin:

$$30^\circ C + 273 = 303 K$$

Determine the molar mass of nitrogen in kilograms:

Extra close brace or missing open brace

Replace the variables and constants in the root-mean-square speed equation, replacing Joules with the equivalent kg $m^2 s^{-2}$:

$$u_{rms} = \sqrt{\frac{3RT}{M}}$$

$$u_{rms} = \sqrt{\frac{3(8.314 J/molK)(303K)}{(0.028 kg/mol)}} = \sqrt{2.70 \times 10^5 m^2 s^{-2}} = 519 m/s$$

Exercise 8.1.1

Calculate the root-mean-square speed for a mole of oxygen molecules at –23 °C.

Answer

441 m/s

If the temperature of a gas increases, its KE_{avg} increases, more molecules have higher speeds and fewer molecules have lower speeds, and the distribution shifts toward higher speeds overall, that is, to the right. If temperature decreases, KE_{avg} decreases, more

molecules have lower speeds and fewer molecules have higher speeds, and the distribution shifts toward lower speeds overall, that is, to the left. This behavior is illustrated for nitrogen gas in Figure 8.1.3.

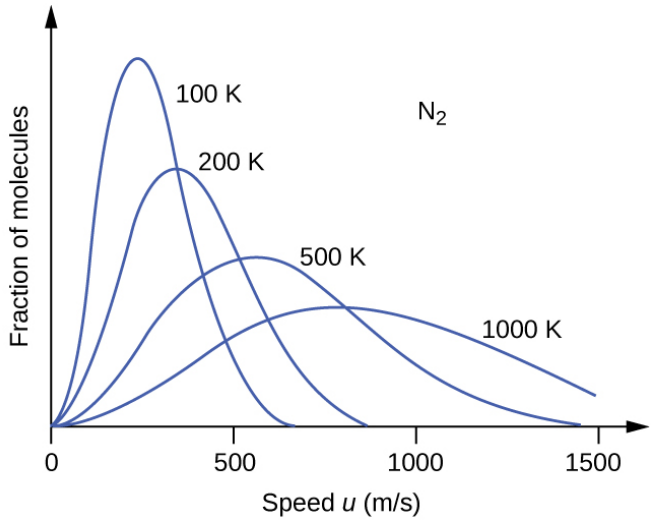


Figure 8.1.3: The molecular speed distribution for nitrogen gas (N_2) shifts to the right and flattens as the temperature increases; it shifts to the left and heightens as the temperature decreases.

At a given temperature, all gases have the same KE_{avg} for their molecules. Gases composed of lighter molecules have more high-speed particles and a higher u_{rms}, with a speed distribution that peaks at relatively higher speeds. Gases consisting of heavier molecules have more low-speed particles, a lower u_{rms}, and a speed distribution that peaks at relatively lower speeds. This trend is demonstrated by the data for a series of noble gases shown in Figure 8.1.4.

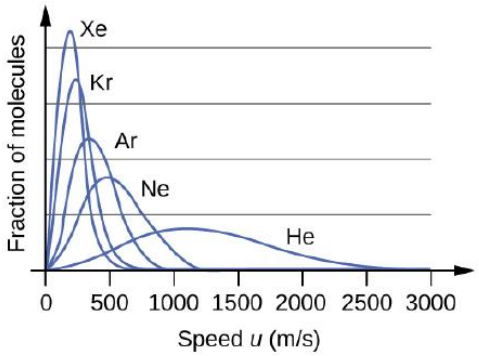


Figure 8.1.4: molecular speed is directly related to molecular mass. At a given temperature, lighter molecules move faster on average than heavier molecules.

Link to Learning

The gas simulator may be used to examine the effect of temperature on molecular speeds. Examine the simulator's "energy histograms" (molecular speed distributions) and "species information" (which gives average speed values) for molecules of different masses at various temperatures.

8.1.3: The Kinetic-Molecular Theory Explains the Behavior of Gases, Part II

According to Graham's law, the molecules of a gas are in rapid motion and the molecules themselves are small. The average distance between the molecules of a gas is large compared to the size of the molecules. As a consequence, gas molecules can move past each other easily and diffuse at relatively fast rates.

The rate of effusion of a gas depends directly on the (average) speed of its molecules:

$$\text{effusion rate} \propto u_{rms}$$

Using this relation, and the equation relating molecular speed to mass, Graham's law may be easily derived as shown here:

$$u_{rms} = \sqrt{\frac{3RT}{M}}$$

$$M = \frac{3RT}{u_{rms}^2} = \frac{3RT}{\bar{u}^2}$$

$$\frac{\text{effusion rate } A}{\text{effusion rate } B} = \frac{u_{rmsA}}{u_{rmsB}} = \frac{\sqrt{\frac{3RT}{M_A}}}{\sqrt{\frac{3RT}{M_B}}} = \sqrt{\frac{M_B}{M_A}}$$

The ratio of the rates of effusion is thus derived to be inversely proportional to the ratio of the square roots of their masses. This is the same relation observed experimentally and expressed as Graham's law.

This page titled 8.1: The Kinetic-Molecular Theory is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **9.5: The Kinetic-Molecular Theory** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.2: Gas Pressure

Learning Objectives

By the end of this section, you will be able to:

- Define the property of pressure
- Define and convert among the units of pressure measurements
- Describe the operation of common tools for measuring gas pressure

The earth's atmosphere exerts a pressure, as does any other gas. Although we do not normally notice atmospheric pressure, we are sensitive to pressure changes—for example, when your ears "pop" during take-off and landing while flying, or when you dive underwater. Gas pressure is caused by the force exerted by gas molecules colliding with the surfaces of objects (Figure **8.2.1**). Although the force of each collision is very small, any surface of appreciable area experiences a large number of collisions in a short time, which can result in a high pressure. In fact, normal air pressure is strong enough to crush a metal container when not balanced by equal pressure from inside the container.

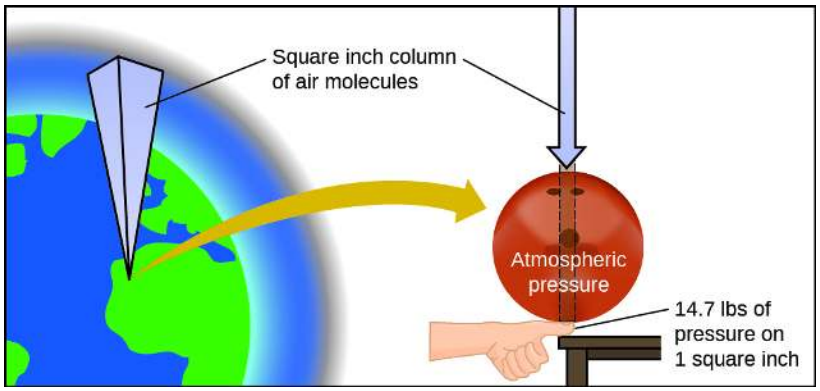


Figure **8.2.1**: The atmosphere above us exerts a large pressure on objects at the surface of the earth, roughly equal to the weight of a bowling ball pressing on an area the size of a human thumbnail.

Link to Learning

A dramatic illustration of atmospheric pressure is provided in this brief video, which shows a railway tanker car imploding when its internal pressure is decreased.

A smaller scale demonstration of this phenomenon is briefly explained.

Atmospheric pressure is caused by the weight of the column of air molecules in the atmosphere above an object, such as the tanker car. At sea level, this pressure is roughly the same as that exerted by a full-grown African elephant standing on a doormat, or a typical bowling ball resting on your thumbnail. These may seem like huge amounts, and they are, but life on earth has evolved under such atmospheric pressure. If you actually perch a bowling ball on your thumbnail, the pressure experienced is *twice* the usual pressure, and the sensation is unpleasant.

In general, **pressure** is defined as the force exerted on a given area: \(P=\frac{F}{A}). Note that pressure is directly proportional to force and inversely proportional to area. Thus, pressure can be increased either by increasing the amount of force or by decreasing the area over which it is applied; pressure can be decreased by decreasing the force or increasing the area.

Let's apply this concept to determine which exerts a greater pressure in Figure **8.2.2** —the elephant or the figure skater? A large African elephant can weigh 7 tons, supported on four feet, each with a diameter of about 1.5 ft (footprint area of 250 in^2), so the pressure exerted by each foot is about 14 lb/in^2:

$$\text{pressure per elephant foot } = 14,000\frac{lb}{\text{elephant}} \times \frac{1 \text{ elephant}}{4 \text{ feet}} \times \frac{1 \text{ foot}}{250in^2} = 14lb/in^2$$

The figure skater weighs about 120 lbs, supported on two skate blades, each with an area of about 2 in^2, so the pressure exerted by each blade is about 30 lb/in^2:

$$\text{pressure per skate blade } = 120\frac{lb}{\text{skater}} \times \frac{1 \text{ skater}}{2 \text{ blades}} \times \frac{1 \text{ blade}}{2 \text{ in}^2} = 30 lb/in^2$$

Even though the elephant is more than one hundred-times heavier than the skater, it exerts less than one-half of the pressure. On the other hand, if the skater removes their skates and stands with bare feet (or regular footwear) on the ice, the larger area over which their weight is applied greatly reduces the pressure exerted:

$$\text{pressure per human foot } = 120\frac{lb}{\text{skater}} \times \frac{1 \text{ skater}}{2 \text{ feet}} \times \frac{1 \text{ foot}}{30 in^2} = 2 lb/in^2$$



Figure **8.2.2**: Although (a) an elephant's weight is large, creating a very large force on the ground, (b) the figure skater exerts a much higher pressure on the ice due to the small surface area of the skates. (credit a: modification of work by Guido da Rozze; credit b: modification of work by Ryosuke Yagi)

The SI unit of pressure is the **pascal (Pa)**, with 1 Pa = 1 N/m^2, where N is the newton, a unit of force defined as 1 kg m/s^2. One pascal is a small pressure; in many cases, it is more convenient to use units of kilopascal (1 kPa = 1000 Pa) or **bar** (1 bar = 100,000 Pa). In the United States, pressure is often measured in pounds of force on an area of one square inch—**pounds per square inch (psi)**—for example, in car tires. Pressure can also be measured using the unit **atmosphere** (atm), which originally represented the average sea level air pressure at the approximate latitude of Paris (45°). Table **8.2.1** provides some information on these and a few other common units for pressure measurements

Table **8.2.1**: Pressure Units

Unit Name and Abbreviation	Definition or Relation to Other Unit
pascal (Pa)	1 Pa = 1 N/m^2 recommended IUPAC unit
kilopascal (kPa)	1 kPa = 1000 Pa
pounds per square inch (psi)	air pressure at sea level is ~14.7 psi
atmosphere (atm)	1 atm = 101,325 Pa = 760 torr air pressure at sea level is ~1 atm
bar (bar, or b)	1 bar = 100,000 Pa (exactly) commonly used in meteorology
millibar (mbar, or mb)	1000 mbar = 1 bar
inches of mercury (in. Hg)	1 in. Hg = 3386 Pa used by aviation industry, also some weather reports
torr	named after Evangelista Torricelli, inventor of the barometer
millimeters of mercury (mm Hg)	1 mm Hg ~1 torr

Example 8.2.1: Conversion of Pressure Units

The United States National Weather Service reports pressure in both inches of Hg and millibars. Convert a pressure of 29.2 in. Hg into:

a. torr
b. atm
c. kPa
d. mbar

Solution

This is a unit conversion problem. The relationships between the various pressure units are given in Table 8.2.1.

a. $$29.2 \text{ in } Hg_g \times \frac{25.4mm}{1im} \times \frac{1 \text{ torr}}{1mmHg_g} = 742 \text{ torr}$$

b. $$742 \text{ torr } \times \frac{1atm}{760 \text{ torr}} = 0.976atm$$

c. $$742 \text{ torr } \times \frac{101.325kPa}{760 \text{ torr}} = 98.9kPa$$

d. $$98.9kPa \times \frac{1000Pa}{1kPa} \times \frac{1bar}{100,000Pa} \times \frac{1000mbar}{1bar} = 989mbar$$

Exercise 8.2.1

A typical barometric pressure in Kansas City is 740 torr. What is this pressure in atmospheres, in millimeters of mercury, in kilopascals, and in bar?

Answer

0.974 atm; 740 mm Hg; 98.7 kPa; 0.987 bar

We can measure atmospheric pressure, the force exerted by the atmosphere on the earth's surface, with a barometer (Figure 8.2.3). A barometer is a glass tube that is closed at one end, filled with a nonvolatile liquid such as mercury, and then inverted and immersed in a container of that liquid. The atmosphere exerts pressure on the liquid outside the tube, the column of liquid exerts pressure inside the tube, and the pressure at the liquid surface is the same inside and outside the tube. The height of the liquid in the tube is therefore proportional to the pressure exerted by the atmosphere.

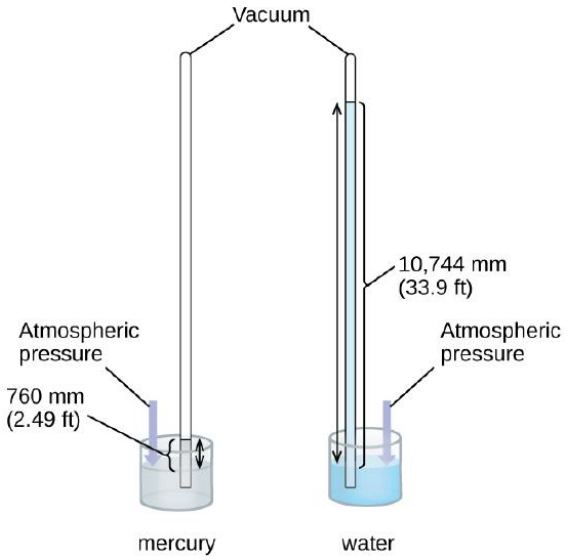


Figure **8.2.3**: In a barometer, the height, *h*, of the column of liquid is used as a measurement of the air pressure. Using very dense liquid mercury (left) permits the construction of reasonably sized barometers, whereas using water (right) would require a barometer more than 30 feet tall.

If the liquid is water, normal atmospheric pressure will support a column of water over 10 meters high, which is rather inconvenient for making (and reading) a barometer. Because mercury (Hg) is about 13.6-times denser than water, a mercury barometer only needs to be Extra close brace or missing open brace as tall as a water barometer—a more suitable size. Standard atmospheric pressure of 1 atm at sea level (101,325 Pa) corresponds to a column of mercury that is about 760 mm (29.92 in.) high. The **torr** was originally intended to be a unit equal to one millimeter of mercury, but it no longer corresponds exactly. The pressure exerted by a fluid due to gravity is known as **hydrostatic pressure**, p:

$$p = h\rho g$$

where h is the height of the fluid, ρ (lowercase Greek letter rho) is the density of the fluid, and g is acceleration due to gravity.

Example 8.2.2: Calculation of Barometric Pressure

Show the calculation supporting the claim that atmospheric pressure near sea level corresponds to the pressure exerted by a column of mercury that is about 760 mm high. The density of mercury = 13.6 g/cm^3.

Solution

The hydrostatic pressure is given by $p = h\rho g$, with h = 760 mm, ρ = 13.6 g/cm^3, and g = 9.81 m/s^2. Plugging these values into the equation and doing the necessary unit conversions will give us the value we seek. (Note: We are expecting to find a pressure of ~101,325 Pa.)

$$101,325 N/m^2 = 101,325 \frac{kg \cdot m/s^2}{m^2} = 101,325 \frac{kg}{m \cdot s^2}$$

$$p = \left(760 mm \times \frac{1m}{1000mm}\right) \times \left(\frac{13.6g}{1cm^3} \times \frac{1kg}{1000g} \times \frac{(100cm)^3}{(1m)^3}\right) \times \left(\frac{9.81m}{1s^2}\right)$$

$$= (0.760m)\left(13,600 kg/m^3\right)\left(9.81 m/s^2\right) = 1.01 \times 10^5 kg/ms^2 = 1.01 \times 10^5 N/m^2$$

$$= 1.01 \times 10^5 Pa$$

Exercise 8.2.2

Calculate the height of a column of water at 25 °C that corresponds to normal atmospheric pressure. The density of water at this temperature is 1.0 g/cm^3.

Answer

10.3 m

A **manometer** is a device similar to a barometer that can be used to measure the pressure of a gas trapped in a container. A closed-end manometer is a U-shaped tube with one closed arm, one arm that connects to the gas to be measured, and a nonvolatile liquid (usually mercury) in between. As with a barometer, the distance between the liquid levels in the two arms of the tube (*h* in the diagram) is proportional to the pressure of the gas in the container. An open-end manometer (Figure **8.2.4**) is the same as a closed-end manometer, but one of its arms is open to the atmosphere. In this case, the distance between the liquid levels corresponds to the difference in pressure between the gas in the container and the atmosphere.

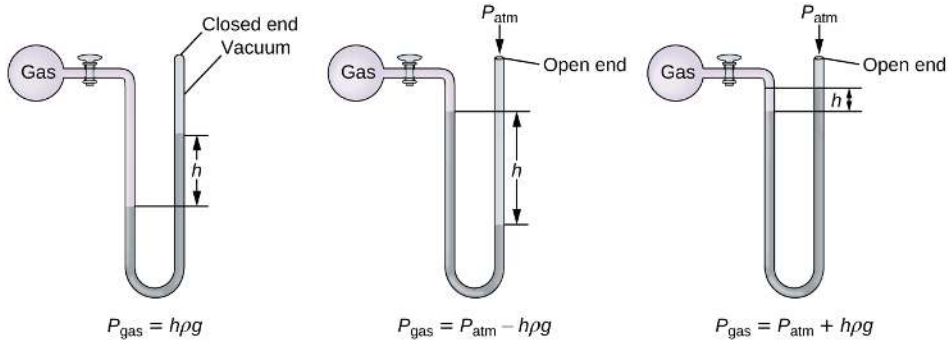
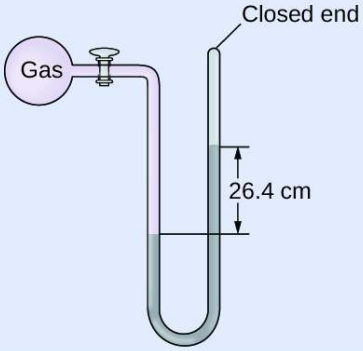


Figure **8.2.4**: A manometer can be used to measure the pressure of a gas. The (difference in) height between the liquid levels (*h*) is a measure of the pressure. Mercury is usually used because of its large density.

Example 8.2.3: Calculation of Pressure Using a Closed-End Manometer

The pressure of a sample of gas is measured with a closed-end manometer, as shown to the right. The liquid in the manometer is mercury. Determine the pressure of the gas in:

a. torr
b. Pa
c. bar



Solution

The pressure of the gas is equal to a column of mercury of height 26.4 cm. (The pressure at the bottom horizontal line is equal on both sides of the tube. The pressure on the left is due to the gas and the pressure on the right is due to 26.4 cm Hg, or mercury.) We could use the equation $p = h\rho g$ as in Example **8.2.2**, but it is simpler to just convert between units using Table **8.2.1**.

a. $$26.4 cm Hg_g \times \frac{10 mm Hg_g}{1 cm Hg} \times \frac{1 \text{ torr}}{1 mm \text{ Hg}} = 264 \text{ torr}$$

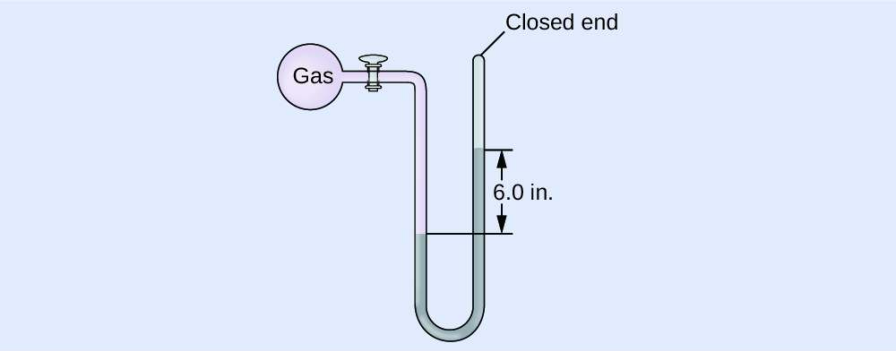
b. $$264 \text{ torr} \times \frac{1 \text{ atm}}{760 \text{ torr}} \times \frac{101,325 Pa}{1 \text{ atm}} = 35,200 Pa$$

c. $$35,200Pa \times \frac{1bar}{100,000Pa} = 0.352bar$$

Exercise 8.2.3

The pressure of a sample of gas is measured with a closed-end manometer. The liquid in the manometer is mercury. Determine the pressure of the gas in:

a. torr
b. Pa
c. bar



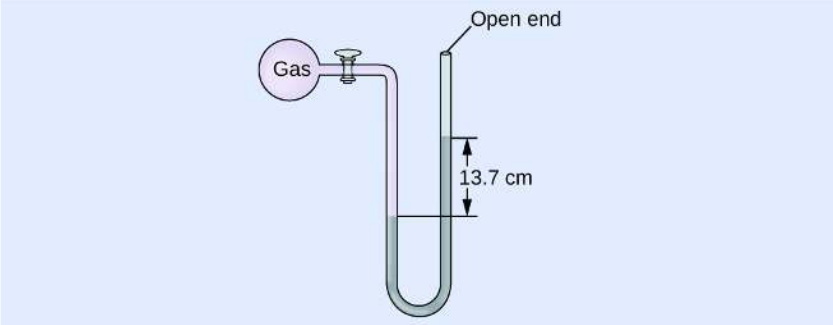
Answer

(a) ~150 torr; (b) ~20,000 Pa; (c) ~0.20 bar

Example 8.2.4: Calculation of Pressure Using an Open-End Manometer

The pressure of a sample of gas is measured at sea level with an open-end Hg (mercury) manometer, as shown to the right. Determine the pressure of the gas in:

a. mm Hg
b. atm
c. kPa



Solution

The pressure of the gas equals the hydrostatic pressure due to a column of mercury of height 13.7 cm plus the pressure of the atmosphere at sea level. (The pressure at the bottom horizontal line is equal on both sides of the tube. The pressure on the left is due to the gas and the pressure on the right is due to 13.7 cm of Hg plus atmospheric pressure.)

a. In mm Hg, this is: 137 mm Hg + 760 mm Hg = 897 mm Hg

b. $$897mmHg_g \times \frac{1atm}{760mmHg_g} = 1.18atm$$

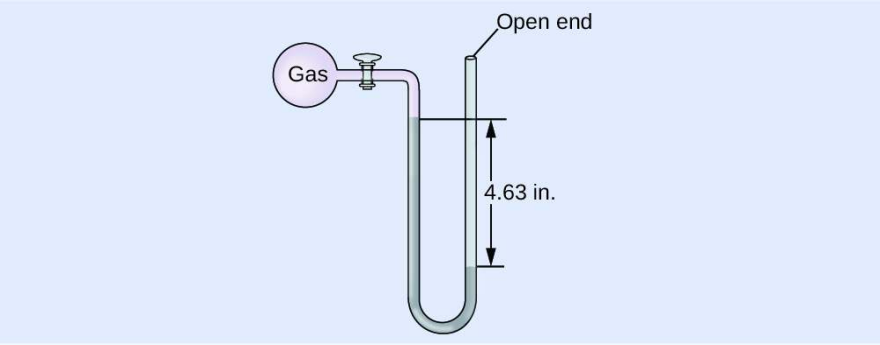
https://chem.libretexts.org/@go/page/449302

c. $$1.18 \text{ atm} \times \frac{101.325 kPa}{1 - 20 \times 10^2 kPa} = 1.20$$

Exercise 8.2.4

The pressure of a sample of gas is measured at sea level with an open-end Hg manometer, as shown to the right. Determine the pressure of the gas in:

a. mm Hg
b. atm
c. kPa



Answer

(a) 642 mm Hg; (b) 0.845 atm; (c) 85.6 kPa

Chemistry in Everyday Life: Measuring Blood Pressure

Blood pressure is measured using a device called a sphygmomanometer (Greek *sphygmos* = "pulse"). It consists of an inflatable cuff to restrict blood flow, a manometer to measure the pressure, and a method of determining when blood flow begins and when it becomes impeded (Figure 8.2.5). Since its invention in 1881, it has been an essential medical device. There are many types of sphygmomanometers: manual ones that require a stethoscope and are used by medical professionals; mercury ones, used when the most accuracy is required; less accurate mechanical ones; and digital ones that can be used with little training but that have limitations. When using a sphygmomanometer, the cuff is placed around the upper arm and inflated until blood flow is completely blocked, then slowly released. As the heart beats, blood forced through the arteries causes a rise in pressure. This rise in pressure at which blood flow begins is the *systolic pressure*—the peak pressure in the cardiac cycle. When the cuff's pressure equals the arterial systolic pressure, blood flows past the cuff, creating audible sounds that can be heard using a stethoscope. This is followed by a decrease in pressure as the heart's ventricles prepare for another beat. As cuff pressure continues to decrease, eventually sound is no longer heard; this is the *diastolic pressure*—the lowest pressure (resting phase) in the cardiac cycle. Blood pressure units from a sphygmomanometer are in terms of millimeters of mercury (mm Hg).



Figure 8.2.5: (a) A medical technician prepares to measure a patient's blood pressure with a sphygmomanometer. (b) A typical sphygmomanometer uses a valved rubber bulb to inflate the cuff and a diaphragm gauge to measure pressure. (credit a: modification of work by Master Sgt. Jeffrey Allen)

How Sciences Interconnect: Meteorology, Climatology, and Atmospheric Science

Throughout the ages, people have observed clouds, winds, and precipitation, trying to discern patterns and make predictions: when it is best to plant and harvest; whether it is safe to set out on a sea voyage; and much more. We now face complex weather and atmosphere-related challenges that will have a major impact on our civilization and the ecosystem. Several different scientific disciplines use chemical principles to help us better understand weather, the atmosphere, and climate. These are meteorology, climatology, and atmospheric science. Meteorology is the study of the atmosphere, atmospheric phenomena, and atmospheric effects on earth's weather. Meteorologists seek to understand and predict the weather in the short term, which can save lives and benefit the economy. Weather forecasts (Figure 8.2.6) are the result of thousands of measurements of air pressure, temperature, and the like, which are compiled, modeled, and analyzed in weather centers worldwide.

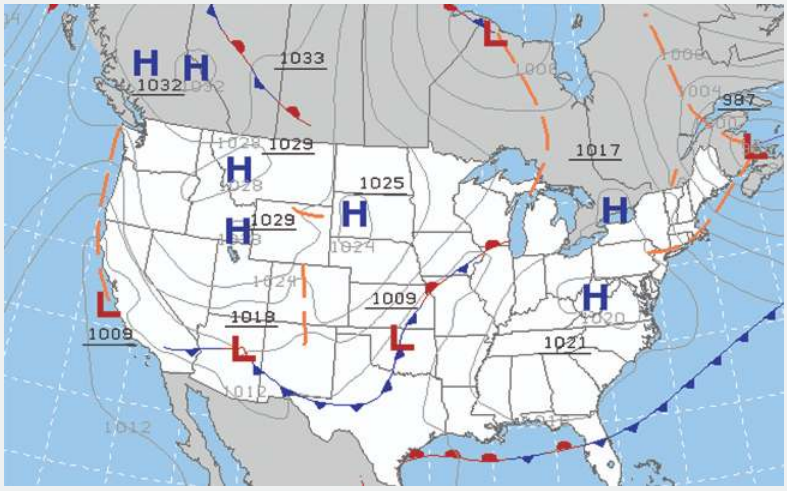


Figure 8.2.6: Meteorologists use weather maps to describe and predict weather. Regions of high (H) and low (L) pressure have large effects on weather conditions. The gray lines represent locations of constant pressure known as isobars. (credit: modification of work by National Oceanic and Atmospheric Administration)

In terms of weather, low-pressure systems occur when the earth's surface atmospheric pressure is lower than the surrounding environment: Moist air rises and condenses, producing clouds. Movement of moisture and air within various weather fronts instigates most weather events.

The atmosphere is the gaseous layer that surrounds a planet. Earth's atmosphere, which is roughly 100–125 km thick, consists of roughly 78.1% nitrogen and 21.0% oxygen, and can be subdivided further into the regions shown in Figure 8.2.7 the exosphere (furthest from earth, > 700 km above sea level), the thermosphere (80–700 km), the mesosphere (50–80 km), the stratosphere (second lowest level of our atmosphere, 12–50 km above sea level), and the troposphere (up to 12 km above sea level, roughly 80% of the earth's atmosphere by mass and the layer where most weather events originate). As you go higher in the troposphere, air density and temperature both decrease.

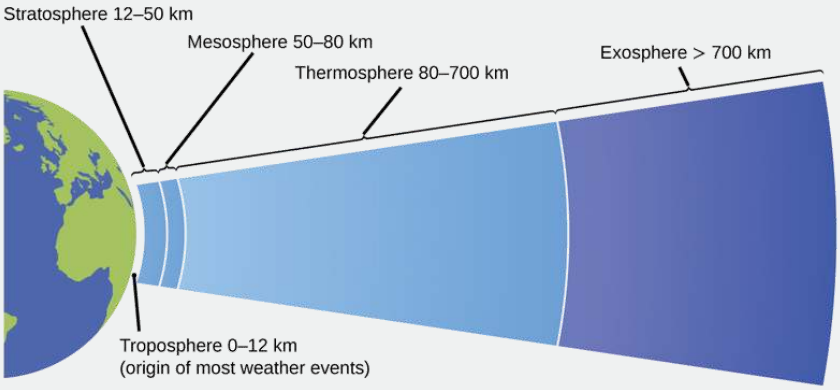


Figure 8.2.7: Earth's atmosphere has five layers: the troposphere, the stratosphere, the mesosphere, the thermosphere, and the exosphere.

Climatology is the study of the climate, averaged weather conditions over long time periods, using atmospheric data. However, climatologists study patterns and effects that occur over decades, centuries, and millennia, rather than shorter time frames of hours, days, and weeks like meteorologists. Atmospheric science is an even broader field, combining meteorology, climatology, and other scientific disciplines that study the atmosphere.

This page titled 8.2: Gas Pressure is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **9.1: Gas Pressure** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.3: The Gas Laws

Learning Objectives

By the end of this section, you will be able to:

- Identify the mathematical relationships between the various properties of gases
- Use the ideal gas law, and related gas laws, to compute the values of various gas properties under specified conditions

During the seventeenth and especially eighteenth centuries, driven both by a desire to understand nature and a quest to make balloons in which they could fly (Figure **8.3.1**), a number of scientists established the relationships between the macroscopic physical properties of gases, that is, pressure, volume, temperature, and amount of gas. Although their measurements were not precise by today's standards, they were able to determine the mathematical relationships between pairs of these variables (e.g., pressure and temperature, pressure and volume) that hold for an *ideal* gas—a hypothetical construct that real gases approximate under certain conditions. Eventually, these individual laws were combined into a single equation—the *ideal gas law*—that relates gas quantities for gases and is quite accurate for low pressures and moderate temperatures. We will consider the key developments in individual relationships (for pedagogical reasons not quite in historical order), then put them together in the ideal gas law.

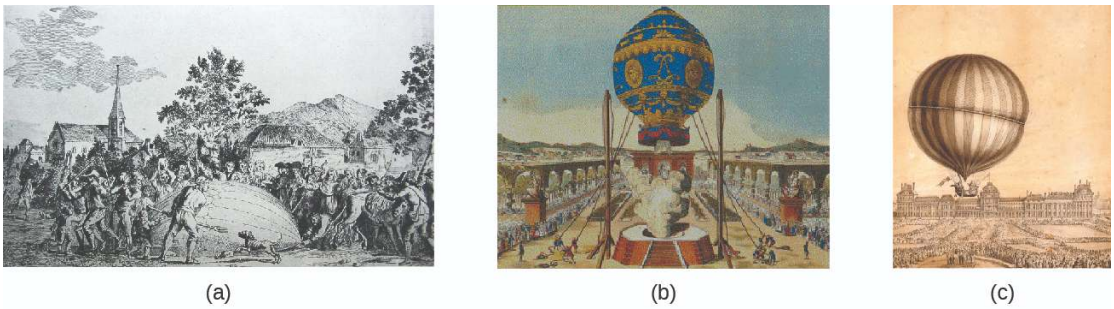


Figure **8.3.1**: In 1783, the first (a) hydrogen-filled balloon flight, (b) manned hot air balloon flight, and (c) manned hydrogen-filled balloon flight occurred. When the hydrogen-filled balloon depicted in (a) landed, the frightened villagers of Gonesse reportedly destroyed it with pitchforks and knives. The launch of the latter was reportedly viewed by 400,000 people in Paris.

8.3.1: Pressure and Temperature: Amontons's Law

Imagine filling a rigid container attached to a pressure gauge with gas and then sealing the container so that no gas may escape. If the container is cooled, the gas inside likewise gets colder and its pressure is observed to decrease. Since the container is rigid and tightly sealed, both the volume and number of moles of gas remain constant. If we heat the sphere, the gas inside gets hotter (Figure **8.3.2**) and the pressure increases.

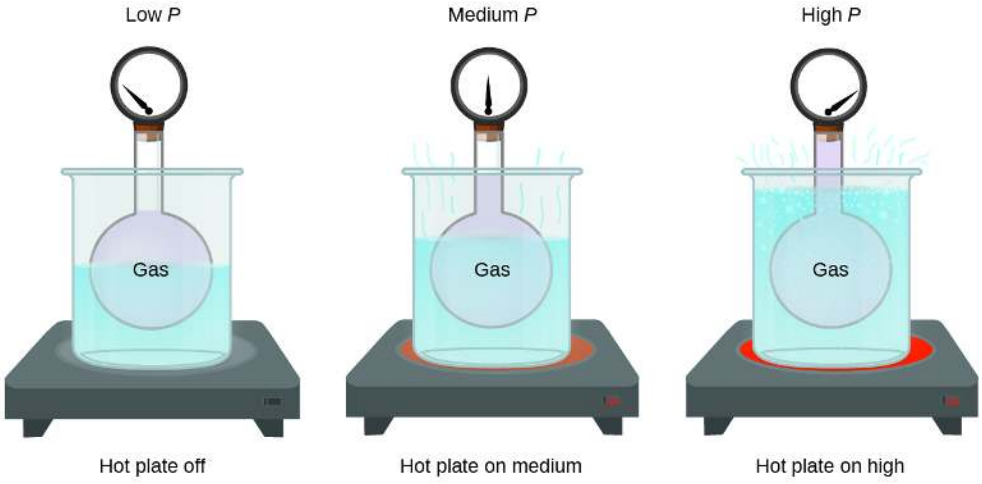


Figure **8.3.2**: The effect of temperature on gas pressure: When the hot plate is off, the pressure of the gas in the sphere is relatively low. As the gas is heated, the pressure of the gas in the sphere increases.

This relationship between temperature and pressure is observed for any sample of gas confined to a constant volume. An example of experimental pressure-temperature data is shown for a sample of air under these conditions in Figure **8.3.3**. We find that temperature and pressure are linearly related, and if the temperature is on the kelvin scale, then P and T are directly proportional (again, when *volume and moles of gas are held constant*); if the temperature on the kelvin scale increases by a certain factor, the gas pressure increases by the same factor.

Temperature (°C)	Temperature (K)	Pressure (kPa)
−100	173	36.0
−50	223	46.4
0	273	56.7
50	323	67.1
100	373	77.5
150	423	88.0

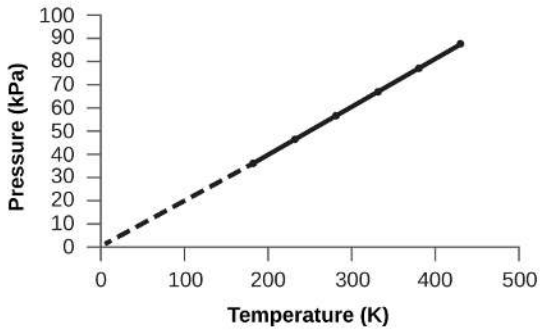


Figure **8.3.3**: For a constant volume and amount of air, the pressure and temperature are directly proportional, provided the temperature is in kelvin. (Measurements cannot be made at lower temperatures because of the condensation of the gas.) When this line is extrapolated to lower pressures, it reaches a pressure of 0 at –273 °C, which is 0 on the kelvin scale and the lowest possible temperature, called absolute zero.

Guillaume Amontons was the first to empirically establish the relationship between the pressure and the temperature of a gas (~1700), and Joseph Louis Gay-Lussac determined the relationship more precisely (~1800). Because of this, the P-T relationship for gases is known as either **Amontons's law** or **Gay-Lussac's law**. Under either name, it states that *the pressure of a given amount of gas is directly proportional to its temperature on the kelvin scale when the volume is held constant*. Mathematically, this can be written:

$$P \propto T \text{ or } P = \text{ constant } \times T \text{ or } P = k \times T$$

where $\propto$ means "is proportional to," and k is a proportionality constant that depends on the identity, amount, and volume of the gas.

For a confined, constant volume of gas, the $\frac{P}{T}$ ratio is therefore constant (i.e., $\frac{P}{T} = k$). If the gas is initially in "Condition 1" (with $P = P_1$ and $T = T_1$), and then changes to "Condition 2" (with $P = P_2$ and $T = T_2$), we have that $\frac{P_1}{T_1} = k$ and $\frac{P_2}{T_2} = k$ which reduces to

$$\frac{P_1}{T_1} = \frac{P_2}{T_2}.$$

This equation is useful for pressure-temperature calculations for a confined gas at constant volume. Note that temperatures must be on the kelvin scale for any gas law calculations (0 on the kelvin scale and the lowest possible temperature is called **absolute zero**). (Also note that there are at least three ways we can describe how the pressure of a gas changes as its temperature changes: We can use a table of values, a graph, or a mathematical equation.)

✔ Example 8.3.1: Predicting Change in Pressure with Temperature

A can of hair spray is used until it is empty except for the propellant, isobutane gas.

a. On the can is the warning "Store only at temperatures below 120 °F (48.8 °C). Do not incinerate." Why?
b. The gas in the can is initially at 24 °C and 360 kPa, and the can has a volume of 350 mL. If the can is left in a car that reaches 50 °C on a hot day, what is the new pressure in the can?

Solution

(a) The can contains an amount of isobutane gas at a constant volume, so if the temperature is increased by heating, the pressure will increase proportionately. High temperature could lead to high pressure, causing the can to burst. (Also, isobutane is combustible, so incineration could cause the can to explode.)

(b) We are looking for a pressure change due to a temperature change at constant volume, so we will use Amontons's/Gay-Lussac's law. Taking P_1 and T_1 as the initial values, T_2 as the temperature where the pressure is unknown and P_2 as the

unknown pressure, and converting °C to K, we have:

$$\frac{P_1}{T_1} = \frac{P_2}{T_2} \text{ which means that } \frac{360 \text{ kPa}}{297 \text{ K}} = \frac{P_2}{323 \text{ K}}$$

Rearranging and solving gives:

$$P_2 = \frac{360 \text{ kPa} \times 323 \cancel{\text{K}}}{297 \cancel{\text{K}}} = 390 \text{ kPa}$$

? Exercise 8.3.1

A sample of nitrogen, N_2, occupies 45.0 mL at 27 °C and 600 torr. What pressure will it have if cooled to –73 °C while the volume remains constant?

Answer

400 torr

8.3.2: Volume and Temperature: Charles's Law

If we fill a balloon with air and seal it, the balloon contains a specific amount of air at atmospheric pressure, let's say 1 atm. If we put the balloon in a refrigerator, the gas inside gets cold and the balloon shrinks (although both the amount of gas and its pressure remain constant). If we make the balloon very cold, it will shrink a great deal, and it expands again when it warms up.

Link to Learning

This video shows how cooling and heating a gas causes its volume to decrease or increase, respectively.

These examples of the effect of temperature on the volume of a given amount of a confined gas at constant pressure are true in general: The volume increases as the temperature increases, and decreases as the temperature decreases. Volume-temperature data for a 1-mole sample of methane gas at 1 atm are listed and graphed in Figure 9.12.

Temperature (°C)	Temperature (K)	Volume (L)
–3	270	22
–23	250	21
–53	220	18
–162	111	9

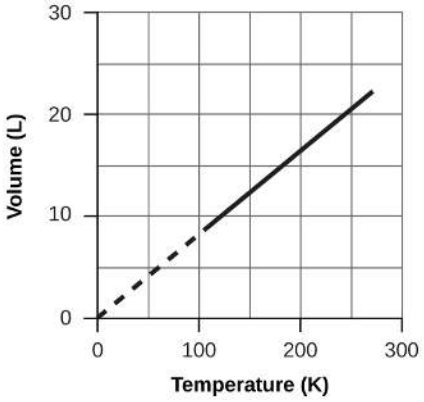


Figure 9.12 The volume and temperature are linearly related for 1 mole of methane gas at a constant pressure of 1 atm. If the temperature is in kelvin, volume and temperature are directly proportional. The line stops at 111 K because methane liquefies at this temperature; when extrapolated, it intersects the graph's origin, representing a temperature of absolute zero.

The relationship between the volume and temperature of a given amount of gas at constant pressure is known as Charles's law in recognition of the French scientist and balloon flight pioneer Jacques Alexandre César Charles. **Charles's law** states that *the volume of a given amount of gas is directly proportional to its temperature on the kelvin scale when the pressure is held constant.*

Mathematically, this can be written as:

$$V \alpha T \text{ or } V = \text{ constant } \cdot T \text{ or } V = k \cdot T \text{ or } V_1/T_1 = V_2/T_2$$

with k being a proportionality constant that depends on the amount and pressure of the gas.

For a confined, constant pressure gas sample, $\frac{V}{T}$ is constant (i.e., the ratio = k), and as seen with the P-T relationship, this leads to another form of Charles's law:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}. \tag{8.3.1}$$

Example 8.3.2: Predicting Change in Volume with Temperature

A sample of carbon dioxide, CO_2, occupies 0.300 L at 10 °C and 750 torr. What volume will the gas have at 30 °C and 750 torr?

Solution

Because we are looking for the volume change caused by a temperature change at constant pressure, this is a job for Charles's law. Taking V_1 and T_1 as the initial values, T_2 as the temperature at which the volume is unknown and V_2 as the unknown volume, and converting °C into K we have:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \text{ which means that } \frac{0.300L}{283K} = \frac{V_2}{303K}$$

Rearranging and solving gives:

$$V_2 = \frac{0.300L \times 303 \cancel{K}}{283 \cancel{K}} = 0.321 \text{ L}$$

This answer supports our expectation from Charles's law, namely, that raising the gas temperature (from 283 K to 303 K) at a constant pressure will yield an increase in its volume (from 0.300 L to 0.321 L).

Exercise 8.3.2

A sample of oxygen, O_2, occupies 32.2 mL at 30 °C and 452 torr. What volume will it occupy at –70 °C and the same pressure?

Answer

21.6 mL

Example 8.3.3: Measuring Temperature with a Volume Change

Temperature is sometimes measured with a gas thermometer by observing the change in the volume of the gas as the temperature changes at constant pressure. The hydrogen in a particular hydrogen gas thermometer has a volume of 150.0 cm^3 when immersed in a mixture of ice and water (0.00 °C). When immersed in boiling liquid ammonia, the volume of the hydrogen, at the same pressure, is 131.7 cm^3. Find the temperature of boiling ammonia on the kelvin and Celsius scales.

Solution

A volume change caused by a temperature change at constant pressure means we should use Charles's law. Taking V_1 and T_1 as the initial values, T_2 as the temperature at which the volume is unknown and V_2 as the unknown volume, and converting °C into K we have:

$$\frac{V_1}{T_1} = \frac{V_2}{T_2} \text{ which means that } \frac{150.0cm^3}{273.15K} = \frac{131.7cm^3}{T_2}$$

Rearrangement gives

$$T_2 = \frac{131.7 \cancel{cm^3} \times 273.15 \text{ K}}{150.0 \cancel{cm^3}} = 239.8 \text{ K}$$

Subtracting 273.15 from 239.8 K, we find that the temperature of the boiling ammonia on the Celsius scale is –33.4 °C.

? Exercise 8.3.3

What is the volume of a sample of ethane at 467 K and 1.1 atm if it occupies 405 mL at 298 K and 1.1 atm?

Answer

635 mL

8.3.3: Volume and Pressure: Boyle's Law

If we partially fill an airtight syringe with air, the syringe contains a specific amount of air at constant temperature, say 25 °C. If we slowly push in the plunger while keeping temperature constant, the gas in the syringe is compressed into a smaller volume and its pressure increases; if we pull out the plunger, the volume increases and the pressure decreases. This example of the effect of volume on the pressure of a given amount of a confined gas is true in general. Decreasing the volume of a contained gas will increase its pressure, and increasing its volume will decrease its pressure. In fact, if the volume increases by a certain factor, the pressure decreases by the same factor, and vice versa. Volume-pressure data for an air sample at room temperature are graphed in Figure **8.3.4**.

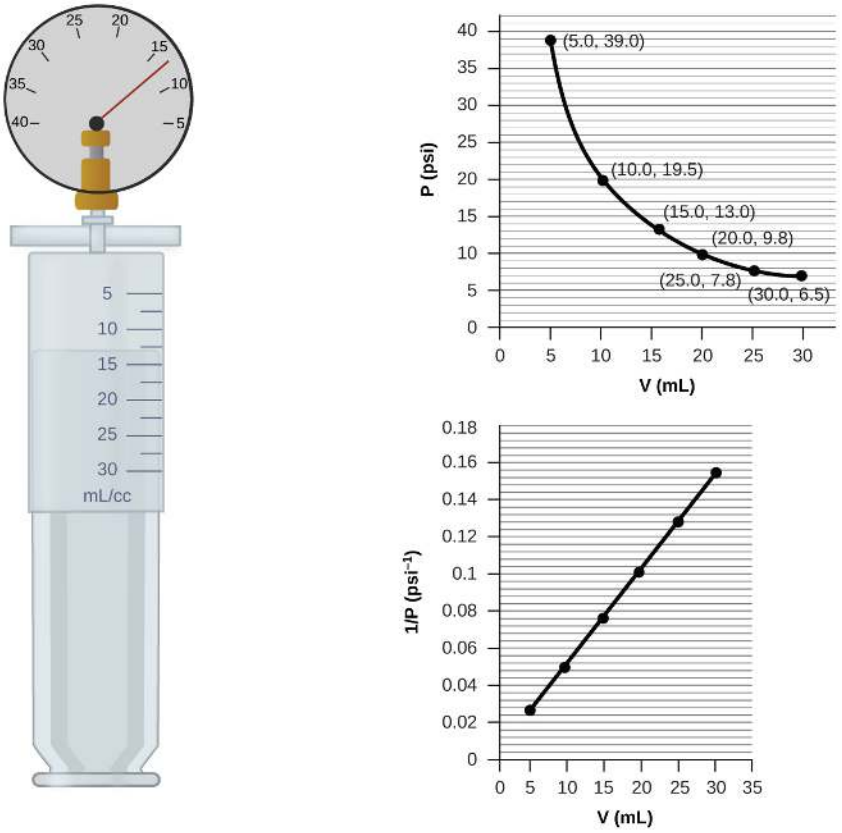


Figure **8.3.4**: When a gas occupies a smaller volume, it exerts a higher pressure; when it occupies a larger volume, it exerts a lower pressure (assuming the amount of gas and the temperature do not change). Since P and V are inversely proportional, a graph of $\frac{1}{P}$ vs. V is linear.

Unlike the P-T and V-T relationships, pressure and volume are not directly proportional to each other. Instead, P and V exhibit inverse proportionality: Increasing the pressure results in a decrease of the volume of the gas. Mathematically this can be written:

$$P \propto \frac{1}{V} \tag{8.3.2}$$

or

$$P = k \cdot \frac{1}{V} \tag{8.3.3}$$

or

$$P \cdot V = k \tag{8.3.4}$$

or

$$P_1V_1 = P_2V_2 \tag{8.3.5}$$

with k being a constant. Graphically, this relationship is shown by the straight line that results when plotting the inverse of the pressure

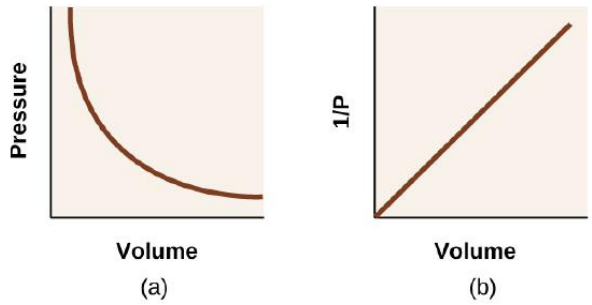


Figure 8.3.5: The relationship between pressure and volume is inversely proportional. (a) The graph of P vs. V is a hyperbola, whereas (b) the graph of $\frac{1}{P}$ vs. V is linear.

The relationship between the volume and pressure of a given amount of gas at constant temperature was first published by the English natural philosopher Robert Boyle over 300 years ago. It is summarized in the statement now known as **Boyle's law**: *The volume of a given amount of gas held at constant temperature is inversely proportional to the pressure under which it is measured.*

Example 8.3.4: Volume of a Gas Sample

The sample of gas in Figure 8.3.4: has a volume of 15.0 mL at a pressure of 13.0 psi. Determine the pressure of the gas at a volume of 7.5 mL, using:

a. the P-V graph in Figure 8.3.5
b. the $\frac{1}{P}$ vs. V graph in Figure 8.3.5
c. the Boyle's law equations (Equations 8.3.2 - 8.3.5)

Comment on the likely accuracy of each method.

Solution

(a) Estimating from the P-V graph gives a value for P somewhere around 27 psi.

(b) Estimating from the \frac{1}{P}\) versus V graph give a value of about 26 psi.

(c) From Boyle's law, we know that the product of pressure and volume (PV) for a given sample of gas at a constant temperature is always equal to the same value. Therefore we have $P_1V_1 = k$ and $P_2V_2 = k$ which means that $P_1V_1 = P_2V_2$.

Using P_1 and V_1 as the known values 13.0 psi and 15.0 mL, P_2 as the pressure at which the volume is unknown, and V_2 as the unknown volume, we have:

$$P_1\ V_1 = P_2\ V_2$$
$$(13.0\ \text{psi}) \times (15.0\ \text{mL} = P_2 \times (7.5\ \text{mL})$$

Solving:

$$P_2 = \frac{13.0\ \text{psi} \times 15.0\ \cancel{\text{mL}}}{7.5\ \cancel{\text{mL}}} = 26\ \text{psi}$$

It was more difficult to estimate well from the P-V graph, so (a) is likely more inaccurate than (b) or (c). The calculation will be as accurate as the equation and measurements allow.

Exercise 8.3.4

The sample of gas in Figure **8.3.4** has a volume of 30.0 mL at a pressure of 6.5 psi. Determine the volume of the gas at a pressure of 11.0 psi, using:

a. the *P*-*V* graph in Figure **8.3.5**
b. the $\frac{1}{P}$ vs. \(*V*\) graph in Figure **8.3.5**
c. the Boyle's law equations (8.3.2 - 8.3.5)

Comment on the likely accuracy of each method.

Answer

(a) about 17–18 mL; (b) ~18 mL; (c) 17.7 mL; it was more difficult to estimate well from the *P*-*V* graph, so (a) is likely more inaccurate than (b); the calculation will be as accurate as the equation and measurements allow

Chemistry in Everyday Life: Breathing and Boyle's Law

What do you do about 20 times per minute for your whole life, without break, and often without even being aware of it? The answer, of course, is respiration, or breathing. How does it work? It turns out that the gas laws apply here. Your lungs take in gas that your body needs (oxygen) and get rid of waste gas (carbon dioxide). Lungs are made of spongy, stretchy tissue that expands and contracts while you breathe. When you inhale, your diaphragm and intercostal muscles (the muscles between your ribs) contract, expanding your chest cavity and making your lung volume larger. The increase in volume leads to a decrease in pressure (Boyle's law). This causes air to flow into the lungs (from high pressure to low pressure). When you exhale, the process reverses: Your diaphragm and rib muscles relax, your chest cavity contracts, and your lung volume decreases, causing the pressure to increase (Boyle's law again), and air flows out of the lungs (from high pressure to low pressure). You then breathe in and out again, and again, repeating this Boyle's law cycle for the rest of your life (Figure **8.3.6**).

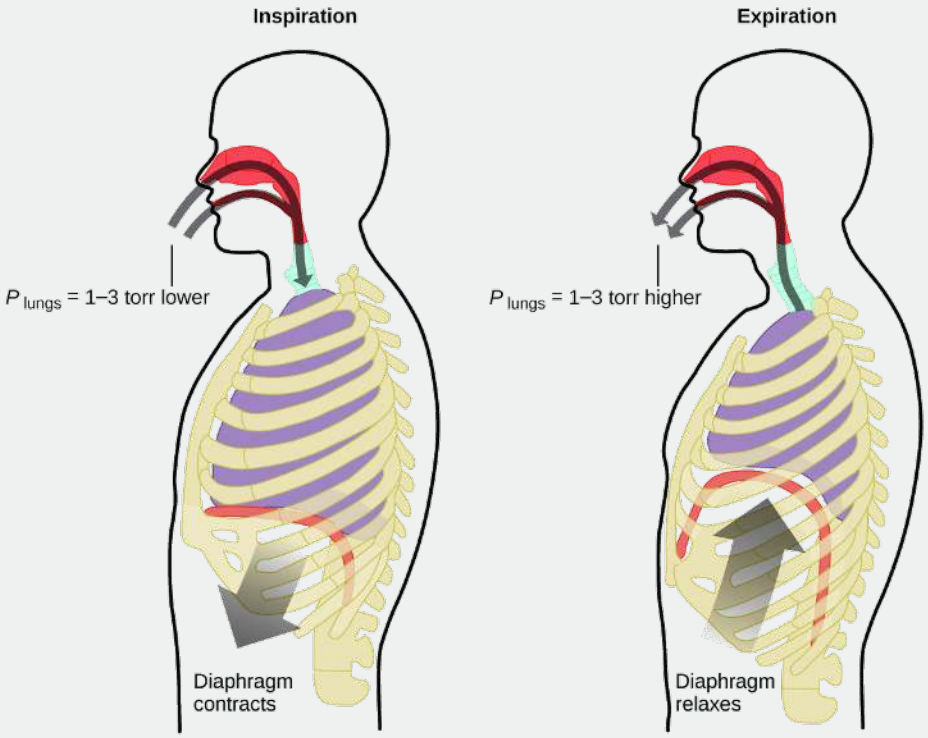


Figure **8.3.6**: Breathing occurs because expanding and contracting lung volume creates small pressure differences between your lungs and your surroundings, causing air to be drawn into and forced out of your lungs.

8.3.4: Moles of Gas and Volume: Avogadro's Law

The Italian scientist Amedeo Avogadro advanced a hypothesis in 1811 to account for the behavior of gases, stating that equal volumes of all gases, measured under the same conditions of temperature and pressure, contain the same number of molecules. Over time, this relationship was supported by many experimental observations as expressed by **Avogadro's law**: *For a confined gas, the volume (V) and number of moles (n) are directly proportional if the pressure and temperature both remain constant.*

In equation form, this is written as:

$$V \propto n \tag{8.3.6}$$

or

$$V = k \times n \tag{8.3.7}$$

or

$$\frac{V_1}{n_1} = \frac{V_2}{n_2} \tag{8.3.8}$$

Mathematical relationships can also be determined for the other variable pairs, such as *P* versus *n*, and *n* versus *T*.

Link to Learning

Visit this interactive PhET simulation to investigate the relationships between pressure, volume, temperature, and amount of gas. Use the simulation to examine the effect of changing one parameter on another while holding the other parameters constant (as described in the preceding sections on the various gas laws).

8.3.5: The Ideal Gas Law

To this point, four separate laws have been discussed that relate pressure, volume, temperature, and the number of moles of the gas:

- Boyle's law: PV = constant at constant T and n
- Amontons's law: $\frac{P}{T}$ = constant at constant V and n
- Charles's law: $\frac{V}{T}$ = constant at constant P and n
- Avogadro's law: $\frac{V}{n}$ = constant at constant P and T

Combining these four laws yields the **ideal gas law**, a relation between the pressure, volume, temperature, and number of moles of a gas:

$$PV = nRT$$

where P is the pressure of a gas, V is its volume, n is the number of moles of the gas, T is its temperature on the kelvin scale, and R is a constant called the **ideal gas constant** or the universal gas constant. The units used to express pressure, volume, and temperature will determine the proper form of the gas constant as required by dimensional analysis, the most commonly encountered values being 0.08206 L atm mol^{-1} K^{-1} and 8.314 kPa L mol^{-1} K^{-1}.

Gases whose properties of P, V, and T are accurately described by the ideal gas law (or the other gas laws) are said to exhibit *ideal behavior* or to approximate the traits of an **ideal gas**. An ideal gas is a hypothetical construct that may be used along with *kinetic molecular theory* to effectively explain the gas laws as will be described in a later module of this chapter. Although all the calculations presented in this module assume ideal behavior, this assumption is only reasonable for gases under conditions of relatively low pressure and high temperature. In the final module of this chapter, a modified gas law will be introduced that accounts for the *non-ideal* behavior observed for many gases at relatively high pressures and low temperatures.

The ideal gas equation contains five terms, the gas constant R and the variable properties P, V, n, and T. Specifying any four of these terms will permit use of the ideal gas law to calculate the fifth term as demonstrated in the following example exercises.

Example 8.3.5: Using the Ideal Gas Law

Methane, CH_4, is being considered for use as an alternative automotive fuel to replace gasoline. One gallon of gasoline could be replaced by 655 g of CH_4. What is the volume of this much methane at 25 °C and 745 torr?

Solution

We must rearrange $PV = nRT$ to solve for V:

$$V = \frac{nRT}{P}$$

If we choose to use R = 0.08206 L atm mol^{-1} K^{-1}, then the amount must be in moles, temperature must be in kelvin, and pressure must be in atm.

Converting into the "right" units:

$$n = 655 \text{ g } CH_4 \times \frac{1 \text{ mol}}{16.043 \text{ g } CH_4} = 40.8 \text{ mol}$$

$$T = 25°C + 273 = 298 \text{ K}$$

$$P = 745 \text{ torr} \times \frac{1 \text{ atm}}{760 \text{ torr}} = 0.980 \text{ atm}$$

$$V = \frac{nRT}{P} = \frac{(40.8 \text{ mol})\left(0.08206 \text{ L atm mol}^{-1}\text{K}^{-1}\right)(298 \text{ K})}{0.980 \text{ atm}} = 1.02 \times 10^3 \text{ L}$$

It would require 1020 L (269 gal) of gaseous methane at about 1 atm of pressure to replace 1 gal of gasoline. It requires a large container to hold enough methane at 1 atm to replace several gallons of gasoline.

Exercise 8.3.5

Calculate the pressure in bar of 2520 moles of hydrogen gas stored at 27 °C in the 180-L storage tank of a modern hydrogen-powered car.

Answer

350 bar

If the number of moles of an ideal gas are kept constant under two different sets of conditions, a useful mathematical relationship called the **combined gas law** is obtained:

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

using units of atm, L, and K. Both sets of conditions are equal to the product of n R (where n = the number of moles of the gas and R is the ideal gas law constant).

Example 8.3.6: Using the Combined Gas Law

When filled with air, a typical scuba tank with a volume of 13.2 L has a pressure of 153 atm (Figure **8.3.7**). If the water temperature is 27 °C, how many liters of air will such a tank provide to a diver's lungs at a depth of approximately 70 feet in the ocean where the pressure is 3.13 atm?



Figure 8.3.7: Scuba divers use compressed air to breathe while underwater. (credit: modification of work by Mark Goodchild)

Letting *1* represent the air in the scuba tank and *2* represent the air in the lungs, and noting that body temperature (the temperature the air will be in the lungs) is 37 °C, we have:

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2} \rightarrow \frac{(153atm)(13.2L)}{(300K)} = \frac{(3.13atm)\,(V_2)}{(310K)}$$

Solving for V_2:

$$V_2 = \frac{(153\text{ atm})(13.2L)(310K)}{(300K)(3.13\text{ atm})} = 667L$$

(Note: Be advised that this particular example is one in which the assumption of ideal gas behavior is not very reasonable, since it involves gases at relatively high pressures and low temperatures. Despite this limitation, the calculated volume can be viewed as a good “ballpark” estimate.)

? Exercise 8.3.6

A sample of ammonia is found to occupy 0.250 L under laboratory conditions of 27 °C and 0.850 atm. Find the volume of this sample at 0 °C and 1.00 atm.

Answer

0.193 L

Chemistry in Everyday Life: The Interdependence between Ocean Depth and Pressure in Scuba Diving

Whether scuba diving at the Great Barrier Reef in Australia (shown in Figure 8.3.8) or in the Caribbean, divers must understand how pressure affects a number of issues related to their comfort and safety.



Figure **8.3.8**: Scuba divers, whether at the Great Barrier Reef or in the Caribbean, must be aware of buoyancy, pressure equalization, and the amount of time they spend underwater, to avoid the risks associated with pressurized gases in the body. (credit: Kyle Taylor)

Pressure increases with ocean depth, and the pressure changes most rapidly as divers reach the surface. The pressure a diver experiences is the sum of all pressures above the diver (from the water and the air). Most pressure measurements are given in units of atmospheres, expressed as “atmospheres absolute” or ATA in the diving community: Every 33 feet of salt water represents 1 ATA of pressure in addition to 1 ATA of pressure from the atmosphere at sea level. As a diver descends, the increase in pressure causes the body’s air pockets in the ears and lungs to compress; on the ascent, the decrease in pressure causes these air pockets to expand, potentially rupturing eardrums or bursting the lungs. Divers must therefore undergo equalization by adding air to body airspaces on the descent by breathing normally and adding air to the mask by breathing out of the nose or adding air to the ears and sinuses by equalization techniques; the corollary is also true on ascent, divers must release air from the body to maintain equalization. Buoyancy, or the ability to control whether a diver sinks or floats, is controlled by the buoyancy compensator (BCD). If a diver is ascending, the air in their BCD expands because of lower pressure according to Boyle’s law (decreasing the pressure of gases increases the volume). The expanding air increases the buoyancy of the diver, and they begin to ascend. The diver must vent air from the BCD or risk an uncontrolled ascent that could rupture the lungs. In descending, the increased pressure causes the air in the BCD to compress and the diver sinks much more quickly; the diver must add air to the BCD or risk an uncontrolled descent, facing much higher pressures near the ocean floor. The pressure also impacts how long a diver can stay underwater before ascending. The deeper a diver dives, the more compressed the air that is breathed because of increased pressure: If a diver dives 33 feet, the pressure is 2 ATA and the air would be compressed to one-half of its original volume. The diver uses up available air twice as fast as at the surface.

8.3.6: Standard Conditions of Temperature and Pressure

We have seen that the volume of a given quantity of gas and the number of molecules (moles) in a given volume of gas vary with changes in pressure and temperature. Chemists sometimes make comparisons against a **standard temperature and pressure (STP)** for reporting properties of gases: 273.15 K and 1 atm (101.325 kPa).[1] At STP, one mole of an ideal gas has a volume of about 22.4 L—this is referred to as the **standard molar volume** (Figure **8.3.9**).

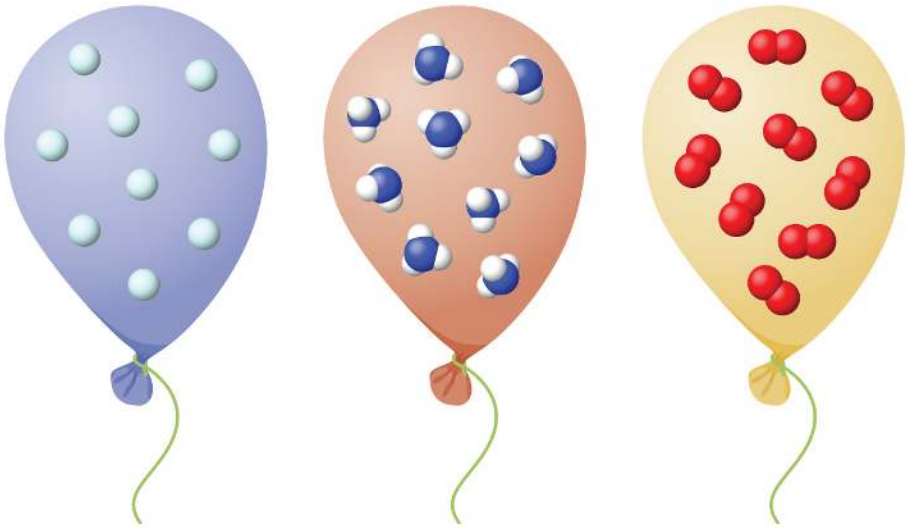


Figure **8.3.9**: Regardless of its chemical identity, one mole of gas behaving ideally occupies a volume of ~22.4 L at STP.

8.3.7: Footnotes

- 1The IUPAC definition of standard pressure was changed from 1 atm to 1 bar (100 kPa) in 1982, but the prior definition remains in use by many literature resources and will be used in this text.

This page titled 8.3: The Gas Laws is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **9.2: Relating Pressure, Volume, Amount, and Temperature - The Ideal Gas Law** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.4: Intermolecular Forces

Learning Objectives

By the end of this section, you will be able to:

- Describe the types of intermolecular forces possible between atoms or molecules in condensed phases (dispersion forces, dipole-dipole attractions, and hydrogen bonding)
- Identify the types of intermolecular forces experienced by specific molecules based on their structures
- Explain the relation between the intermolecular forces present within a substance and the temperatures associated with changes in its physical state

As was the case for gaseous substances, the kinetic molecular theory may be used to explain the behavior of solids and liquids. In the following description, the term *particle* will be used to refer to an atom, molecule, or ion. Note that we will use the popular phrase "intermolecular attraction" to refer to attractive forces between the particles of a substance, regardless of whether these particles are molecules, atoms, or ions.

Consider these two aspects of the molecular-level environments in solid, liquid, and gaseous matter:

- Particles in a solid are tightly packed together and often arranged in a regular pattern; in a liquid, they are close together with no regular arrangement; in a gas, they are far apart with no regular arrangement.
- Particles in a solid vibrate about fixed positions and do not generally move in relation to one another; in a liquid, they move past each other but remain in essentially constant contact; in a gas, they move independently of one another except when they collide.

The differences in the properties of a solid, liquid, or gas reflect the strengths of the attractive forces between the atoms, molecules, or ions that make up each phase. The phase in which a substance exists depends on the relative extents of its **intermolecular forces** (IMFs) and the kinetic energies (KE) of its molecules. IMFs are the various forces of attraction that may exist between the atoms and molecules of a substance due to electrostatic phenomena, as will be detailed in this module. These forces serve to hold particles close together, whereas the particles' KE provides the energy required to overcome the attractive forces and thus increase the distance between particles. Figure 8.4.1 illustrates how changes in physical state may be induced by changing the temperature, hence, the average KE, of a given substance.

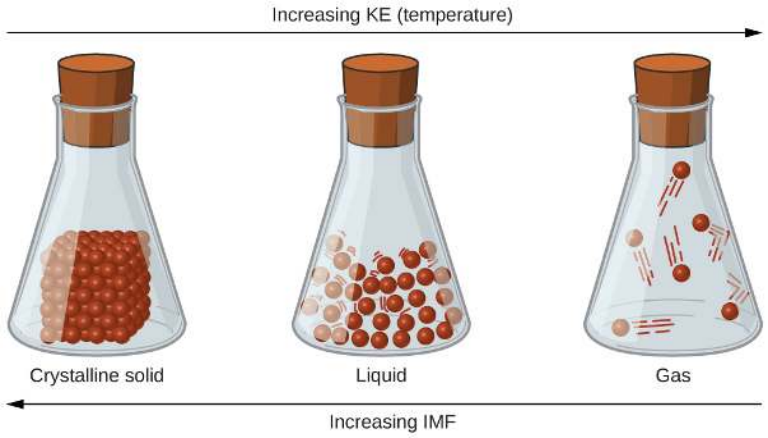


Figure 8.4.1: Transitions between solid, liquid, and gaseous states of a substance occur when conditions of temperature or pressure favor the associated changes in intermolecular forces. (Note: The space between particles in the gas phase is much greater than shown.)

As an example of the processes depicted in this figure, consider a sample of water. When gaseous water is cooled sufficiently, the attractions between H_2O molecules will be capable of holding them together when they come into contact with each other; the gas condenses, forming liquid H_2O. For example, liquid water forms on the outside of a cold glass as the water vapor in the air is cooled by the cold glass, as seen in Figure 8.4.2.



Figure **8.4.2**: Condensation forms when water vapor in the air is cooled enough to form liquid water, such as (a) on the outside of a cold beverage glass or (b) in the form of fog. (credit a: modification of work by Jenny Downing; credit b: modification of work by Cory Zanker)

We can also liquefy many gases by compressing them, if the temperature is not too high. The increased pressure brings the molecules of a gas closer together, such that the attractions between the molecules become strong relative to their KE. Consequently, they form liquids. Butane, C_4H_{10}, is the fuel used in disposable lighters and is a gas at standard temperature and pressure. Inside the lighter's fuel compartment, the butane is compressed to a pressure that results in its condensation to the liquid state, as shown in Figure **8.4.3**.



Figure **8.4.3**: Gaseous butane is compressed within the storage compartment of a disposable lighter, resulting in its condensation to the liquid state. (credit: modification of work by "Sam-Cat"/Flickr)

Finally, if the temperature of a liquid becomes sufficiently low, or the pressure on the liquid becomes sufficiently high, the molecules of the liquid no longer have enough KE to overcome the IMF between them, and a solid forms. A more thorough discussion of these and other changes of state, or phase transitions, is provided in a later module of this chapter.

Link to Learning

Access this interactive simulation on states of matter, phase transitions, and intermolecular forces. This simulation is useful for visualizing concepts introduced throughout this chapter.

8.4.1: Forces between Molecules

Under appropriate conditions, the attractions between all gas molecules will cause them to form liquids or solids. This is due to intermolecular forces, not *intra*molecular forces. *Intra*molecular forces are those *within* the molecule that keep the molecule together, for example, the bonds between the atoms. *Inter*molecular forces are the attractions *between* molecules, which determine many of the physical properties of a substance. Figure **8.4.4**: illustrates these different molecular forces. The strengths of these attractive forces vary widely, though usually the IMFs between small molecules are weak compared to the intramolecular forces that bond atoms together within a molecule. For example, to overcome the IMFs in one mole of liquid HCl and convert it into gaseous HCl requires only about 17 kilojoules. However, to break the covalent bonds between the hydrogen and chlorine atoms in one mole of HCl requires about 25 times more energy—430 kilojoules.

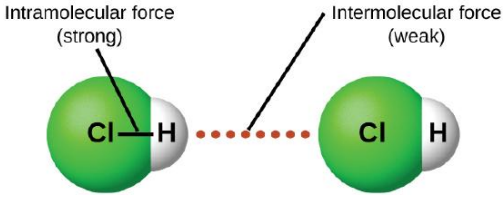


Figure 8.4.4: *Intra*molecular forces keep a molecule intact. *Inter*molecular forces hold multiple molecules together and determine many of a substance's properties.

All of the attractive forces between neutral atoms and molecules are known as van der Waals forces, although they are usually referred to more informally as intermolecular attraction. We will consider the various types of IMFs in the next three sections of this module.

8.4.2: Dispersion Forces

One of the three van der Waals forces is present in all condensed phases, regardless of the nature of the atoms or molecules composing the substance. This attractive force is called the London dispersion force in honor of German-born American physicist Fritz London who, in 1928, first explained it. This force is often referred to as simply the **dispersion force**. Because the electrons of an atom or molecule are in constant motion (or, alternatively, the electron's location is subject to quantum-mechanical variability), at any moment in time, an atom or molecule can develop a temporary, **instantaneous dipole** if its electrons are distributed asymmetrically. The presence of this dipole can, in turn, distort the electrons of a neighboring atom or molecule, producing an **induced dipole**. These two rapidly fluctuating, temporary dipoles thus result in a relatively weak electrostatic attraction between the species—a so-called dispersion force like that illustrated in Figure 8.4.5.

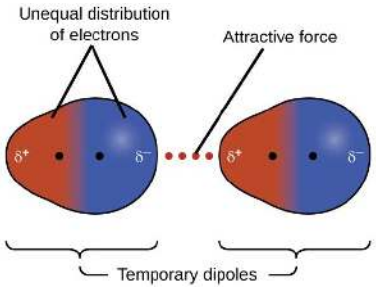


Figure 8.4.5: Dispersion forces result from the formation of temporary dipoles, as illustrated here for two nonpolar diatomic molecules.

Dispersion forces that develop between atoms in different molecules can attract the two molecules to each other. The forces are relatively weak, however, and become significant only when the molecules are very close. Larger and heavier atoms and molecules exhibit stronger dispersion forces than do smaller and lighter atoms and molecules. F_2 and Cl_2 are gases at room temperature (reflecting weaker attractive forces); Br_2 is a liquid, and I_2 is a solid (reflecting stronger attractive forces). Trends in observed melting and boiling points for the halogens clearly demonstrate this effect, as seen in Table 8.4.1.

Table 8.4.1: Melting and Boiling Points of the Halogens

Halogen	Molar Mass	Atomic Radius	Melting Point	Boiling Point
fluorine, F_2	38 g/mol	72 pm	53 K	85 K
chlorine, Cl_2	71 g/mol	99 pm	172 K	238 K
bromine, Br_2	160 g/mol	114 pm	266 K	332 K
iodine, I_2	254 g/mol	133 pm	387 K	457 K
astatine, At_2	420 g/mol	150 pm	575 K	610 K

The increase in melting and boiling points with increasing atomic/molecular size may be rationalized by considering how the strength of dispersion forces is affected by the electronic structure of the atoms or molecules in the substance. In a larger atom, the valence electrons are, on average, farther from the nuclei than in a smaller atom. Thus, they are less tightly held and can more

easily form the temporary dipoles that produce the attraction. The measure of how easy or difficult it is for another electrostatic charge (for example, a nearby ion or polar molecule) to distort a molecule's charge distribution (its electron cloud) is known as polarizability. A molecule that has a charge cloud that is easily distorted is said to be very polarizable and will have large dispersion forces; one with a charge cloud that is difficult to distort is not very polarizable and will have small dispersion forces.

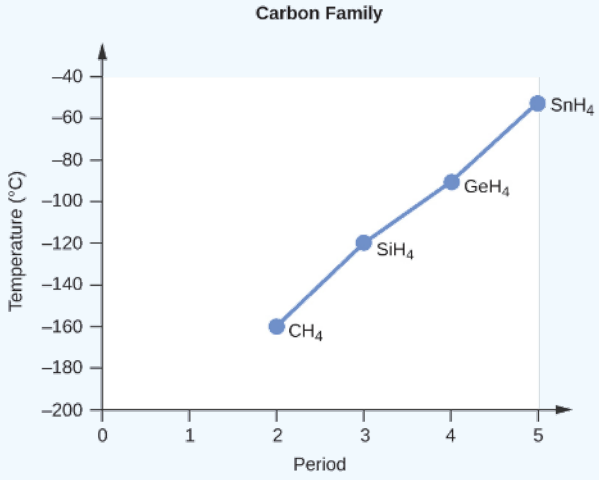
Example 8.4.1: London Forces and Their Effects

Order the following compounds of a group 14 element and hydrogen from lowest to highest boiling point: CH_4, SiH_4, GeH_4, and SnH_4. Explain your reasoning.

Solution

Applying the skills acquired in the chapter on chemical bonding and molecular geometry, all of these compounds are predicted to be nonpolar, so they may experience only dispersion forces: the smaller the molecule, the less polarizable and the weaker the dispersion forces; the larger the molecule, the larger the dispersion forces. The molar masses of CH_4, SiH_4, GeH_4, and SnH_4 are approximately 16 g/mol, 32 g/mol, 77 g/mol, and 123 g/mol, respectively. Therefore, CH_4 is expected to have the lowest boiling point and SnH_4 the highest boiling point. The ordering from lowest to highest boiling point is expected to be $CH_4 < SiH_4 < GeH_4 < SnH_4$.

A graph of the actual boiling points of these compounds versus the period of the group 14 element shows this prediction to be correct:



Exercise 8.4.1

Order the following hydrocarbons from lowest to highest boiling point: C_2H_6, C_3H_8, and C_4H_{10}.

Answer

$C_2H_6 < C_3H_8 < C_4H_{10}$. All of these compounds are nonpolar and only have London dispersion forces: the larger the molecule, the larger the dispersion forces and the higher the boiling point. The ordering from lowest to highest boiling point is therefore $C_2H_6 < C_3H_8 < C_4H_{10}$.

The shapes of molecules also affect the magnitudes of the dispersion forces between them. For example, boiling points for the isomers *n*-pentane, isopentane, and neopentane (shown in Figure **8.4.6**) are 36 °C, 27 °C, and 9.5 °C, respectively. Even though these compounds are composed of molecules with the same chemical formula, C_5H_{12}, the difference in boiling points suggests that dispersion forces in the liquid phase are different, being greatest for *n*-pentane and least for neopentane. The elongated shape of *n*-pentane provides a greater surface area available for contact between molecules, resulting in correspondingly stronger dispersion forces. The more compact shape of isopentane offers a smaller surface area available for intermolecular contact and, therefore, weaker dispersion forces. Neopentane molecules are the most compact of the three, offering the least available surface area for

intermolecular contact and, hence, the weakest dispersion forces. This behavior is analogous to the connections that may be formed between strips of VELCRO brand fasteners: the greater the area of the strip's contact, the stronger the connection.

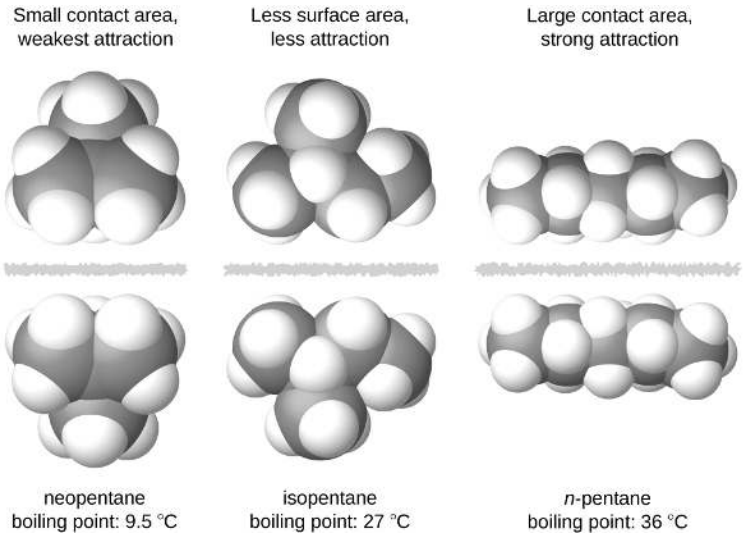


Figure **8.4.6**: The strength of the dispersion forces increases with the contact area between molecules, as demonstrated by the boiling points of these pentane isomers.

Chemistry in Everyday Life: Geckos and Intermolecular Forces

Geckos have an amazing ability to adhere to most surfaces. They can quickly run up smooth walls and across ceilings that have no toe-holds, and they do this without having suction cups or a sticky substance on their toes. And while a gecko can lift its feet easily as it walks along a surface, if you attempt to pick it up, it sticks to the surface. How are geckos (as well as spiders and some other insects) able to do this? Although this phenomenon has been investigated for hundreds of years, scientists only recently uncovered the details of the process that allows geckos' feet to behave this way.

Geckos' toes are covered with hundreds of thousands of tiny hairs known as *setae*, with each seta, in turn, branching into hundreds of tiny, flat, triangular tips called *spatulae*. The huge numbers of spatulae on its setae provide a gecko, shown in Figure **8.4.7**, with a large total surface area for sticking to a surface. In 2000, Kellar Autumn, who leads a multi-institutional gecko research team, found that geckos adhered equally well to both polar silicon dioxide and nonpolar gallium arsenide. This proved that geckos stick to surfaces because of dispersion forces—weak intermolecular attractions arising from temporary, synchronized charge distributions between adjacent molecules. Although dispersion forces are very weak, the total attraction over millions of spatulae is large enough to support many times the gecko's weight.

In 2014, two scientists developed a model to explain how geckos can rapidly transition from "sticky" to "non-sticky." Alex Greaney and Congcong Hu at Oregon State University described how geckos can achieve this by changing the angle between their spatulae and the surface. Geckos' feet, which are normally nonsticky, become sticky when a small shear force is applied. By curling and uncurling their toes, geckos can alternate between sticking and unsticking from a surface, and thus easily move across it. Later research led by Alyssa Stark at University of Akron showed that geckos can maintain their hold on hydrophobic surfaces (similar to the leaves in their habitats) equally well whether the surfaces were wet or dry. Stark's experiment used a ribbon to gently pull the geckos until they slipped, so that the researchers could determine the geckos' ability to hold various surfaces under wet and dry conditions. Further investigations may eventually lead to the development of better adhesives and other applications.

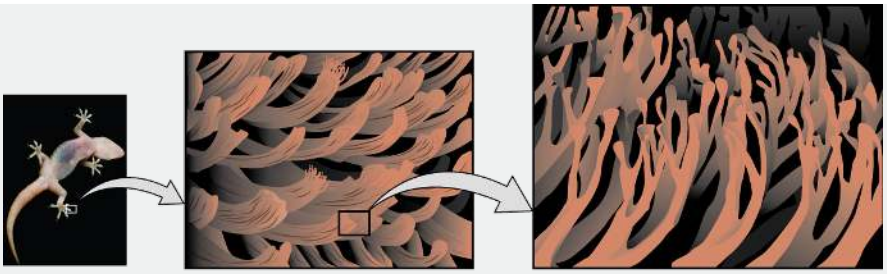


Figure 8.4.7: Geckos' toes contain large numbers of tiny hairs (setae), which branch into many triangular tips (spatulae). Geckos adhere to surfaces because of van der Waals attractions between the surface and a gecko's millions of spatulae. By changing how the spatulae contact the surface, geckos can turn their stickiness "on" and "off." (credit photo: modification of work by "JC*+A!"/Flickr)

Link to Learning

Watch this video to learn more about Kellar Autumn's research that determined that van der Waals forces are responsible for a gecko's ability to cling and climb.

8.4.3: Dipole-Dipole Attractions

Recall from the chapter on chemical bonding and molecular geometry that *polar* molecules have a partial positive charge on one side and a partial negative charge on the other side of the molecule—a separation of charge called a *dipole*. Consider a polar molecule such as hydrogen chloride, HCl. In the HCl molecule, the more electronegative Cl atom bears the partial negative charge, whereas the less electronegative H atom bears the partial positive charge. An attractive force between HCl molecules results from the attraction between the positive end of one HCl molecule and the negative end of another. This attractive force is called a dipole-dipole attraction—the electrostatic force between the partially positive end of one polar molecule and the partially negative end of another, as illustrated in Figure 8.4.8.

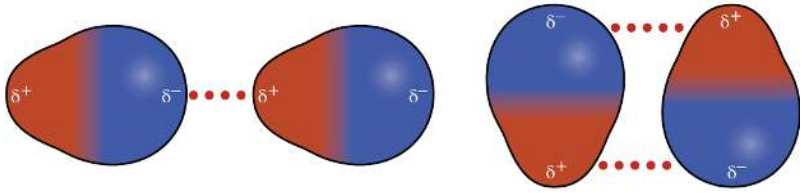


Figure 8.4.8: This image shows two arrangements of polar molecules, such as HCl, that allow an attraction between the partial negative end of one molecule and the partial positive end of another.

The effect of a dipole-dipole attraction is apparent when we compare the properties of HCl molecules to nonpolar F_2 molecules. Both HCl and F_2 consist of the same number of atoms and have approximately the same molecular mass. At a temperature of 150 K, molecules of both substances would have the same average KE. However, the dipole-dipole attractions between HCl molecules are sufficient to cause them to "stick together" to form a liquid, whereas the relatively weaker dispersion forces between nonpolar F_2 molecules are not, and so this substance is gaseous at this temperature. The higher normal boiling point of HCl (188 K) compared to F_2 (85 K) is a reflection of the greater strength of dipole-dipole attractions between HCl molecules, compared to the attractions between nonpolar F_2 molecules. We will often use values such as boiling or freezing points, or enthalpies of vaporization or fusion, as indicators of the relative strengths of IMFs of attraction present within different substances.

Example 8.4.2: Dipole-Dipole Forces and Their Effects

Predict which will have the higher boiling point: N_2 or CO. Explain your reasoning.

Solution

CO and N_2 are both diatomic molecules with masses of about 28 amu, so they experience similar London dispersion forces. Because CO is a polar molecule, it experiences dipole-dipole attractions. Because N_2 is nonpolar, its molecules cannot exhibit

dipole-dipole attractions. The dipole-dipole attractions between CO molecules are comparably stronger than the dispersion forces between nonpolar N_2 molecules, so CO is expected to have the higher boiling point.

? Exercise 8.4.2

Predict which will have the higher boiling point: ICl or Br_2. Explain your reasoning.

Answer

ICl. ICl and Br_2 have similar masses (~160 amu) and therefore experience similar London dispersion forces. ICl is polar and thus also exhibits dipole-dipole attractions; Br_2 is nonpolar and does not. The relatively stronger dipole-dipole attractions require more energy to overcome, so ICl will have the higher boiling point.

8.4.4: Hydrogen Bonding

Nitrosyl fluoride (ONF, molecular mass 49 amu) is a gas at room temperature. Water (H_2O, molecular mass 18 amu) is a liquid, even though it has a lower molecular mass. We clearly cannot attribute this difference between the two compounds to dispersion forces. Both molecules have about the same shape and ONF is the heavier and larger molecule. It is, therefore, expected to experience more significant dispersion forces. Additionally, we cannot attribute this difference in boiling points to differences in the dipole moments of the molecules. Both molecules are polar and exhibit comparable dipole moments. The large difference between the boiling points is due to a particularly strong dipole-dipole attraction that may occur when a molecule contains a hydrogen atom bonded to a fluorine, oxygen, or nitrogen atom (the three most electronegative elements). The very large difference in electronegativity between the H atom (2.1) and the atom to which it is bonded (4.0 for an F atom, 3.5 for an O atom, or 3.0 for a N atom), combined with the very small size of a H atom and the relatively small sizes of F, O, or N atoms, leads to *highly concentrated partial charges* with these atoms. Molecules with F-H, O-H, or N-H moieties are very strongly attracted to similar moieties in nearby molecules, a particularly strong type of dipole-dipole attraction called hydrogen bonding. Examples of hydrogen bonds include HF···HF, H_2O···HOH, and H_3N···HNH_2, in which the hydrogen bonds are denoted by dots. Figure **8.4.9** illustrates hydrogen bonding between water molecules.

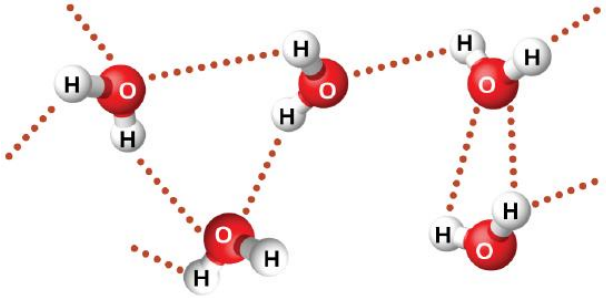


Figure **8.4.9**: Water molecules participate in multiple hydrogen-bonding interactions with nearby water molecules.

Despite use of the word “bond,” keep in mind that hydrogen bonds are *intermolecular* attractive forces, not *intramolecular* attractive forces (covalent bonds). Hydrogen bonds are much weaker than covalent bonds, only about 5 to 10% as strong, but are generally much stronger than other dipole-dipole attractions and dispersion forces.

Hydrogen bonds have a pronounced effect on the properties of condensed phases (liquids and solids). For example, consider the trends in boiling points for the binary hydrides of group 15 (NH_3, PH_3, AsH_3, and SbH_3), group 16 hydrides (H_2O, H_2S, H_2Se, and H_2Te), and group 17 hydrides (HF, HCl, HBr, and HI). The boiling points of the heaviest three hydrides for each group are plotted in Figure **8.4.10**. As we progress down any of these groups, the polarities of the molecules decrease slightly, whereas the sizes of the molecules increase substantially. The effect of increasingly stronger dispersion forces dominates that of increasingly weaker dipole-dipole attractions, and the boiling points are observed to increase steadily.

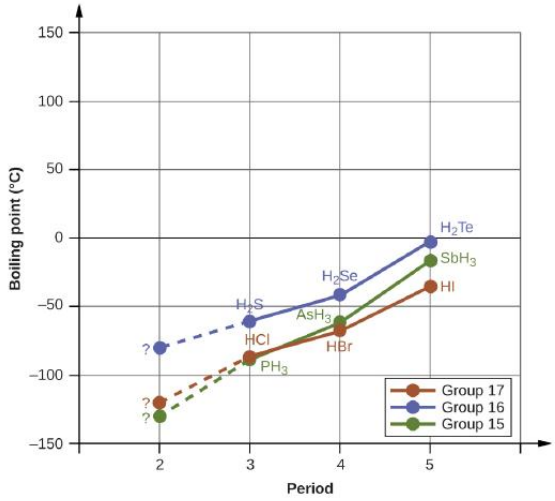


Figure 8.4.10: For the group 15, 16, and 17 hydrides, the boiling points for each class of compounds increase with increasing molecular mass for elements in periods 3, 4, and 5.

If we use this trend to predict the boiling points for the lightest hydride for each group, we would expect NH_3 to boil at about −120 °C, H_2O to boil at about −80 °C, and HF to boil at about −110 °C. However, when we measure the boiling points for these compounds, we find that they are dramatically higher than the trends would predict, as shown in Figure 8.4.11. The stark contrast between our naïve predictions and reality provides compelling evidence for the strength of hydrogen bonding.

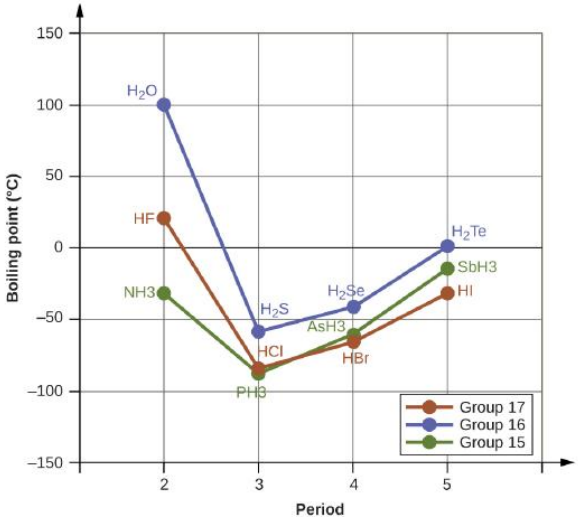


Figure 8.4.11: In comparison to periods 3−5, the binary hydrides of period 2 elements in groups 17, 16 and 15 (F, O and N, respectively) exhibit anomalously high boiling points due to hydrogen bonding.

Example 8.4.3: Effect of Hydrogen Bonding on Boiling Points

Consider the compounds dimethylether (CH_3OCH_3), ethanol (CH_3CH_2OH), and propane ($CH_3CH_2CH_3$). Their boiling points, not necessarily in order, are −42.1 °C, −24.8 °C, and 78.4 °C. Match each compound with its boiling point. Explain your reasoning.

Solution

The VSEPR-predicted shapes of CH_3OCH_3, CH_3CH_2OH, and $CH_3CH_2CH_3$ are similar, as are their molar masses (46 g/mol, 46 g/mol, and 44 g/mol, respectively), so they will exhibit similar dispersion forces. Since $CH_3CH_2CH_3$ is nonpolar, it may exhibit *only* dispersion forces. Because CH_3OCH_3 is polar, it will also experience dipole-dipole attractions. Finally, CH_3CH_2OH has an −OH group, and so it will experience the uniquely strong dipole-dipole attraction known as hydrogen bonding. So the ordering in terms of strength of IMFs, and thus boiling points, is $CH_3CH_2CH_3 < CH_3OCH_3 < CH_3CH_2OH$.

The boiling point of propane is −42.1 °C, the boiling point of dimethylether is −24.8 °C, and the boiling point of ethanol is 78.5 °C.

Exercise 8.4.3

Ethane (CH_3CH_3) has a melting point of −183 °C and a boiling point of −89 °C. Predict the melting and boiling points for methylamine (CH_3NH_2). Explain your reasoning.

Answer

The melting point and boiling point for methylamine are predicted to be significantly greater than those of ethane. CH_3CH_3 and CH_3NH_2 are similar in size and mass, but methylamine possesses an −NH group and therefore may exhibit hydrogen bonding. This greatly increases its IMFs, and therefore its melting and boiling points. It is difficult to predict values, but the known values are a melting point of −93 °C and a boiling point of −6 °C.

How Sciences Interconnect: Hydrogen Bonding and DNA

Deoxyribonucleic acid (DNA) is found in every living organism and contains the genetic information that determines the organism's characteristics, provides the blueprint for making the proteins necessary for life, and serves as a template to pass this information on to the organism's offspring. A DNA molecule consists of two (anti-)parallel chains of repeating nucleotides, which form its well-known double helical structure, as shown in Figure 8.4.12.

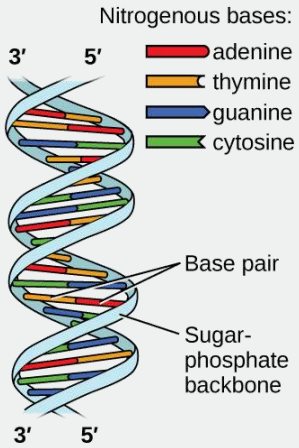


Figure 8.4.12: Two separate DNA molecules form a double-stranded helix in which the molecules are held together via hydrogen bonding. (credit: modification of work by Jerome Walker, Dennis Myts)

Each nucleotide contains a (deoxyribose) sugar bound to a phosphate group on one side, and one of four nitrogenous bases on the other. Two of the bases, cytosine (C) and thymine (T), are single-ringed structures known as pyrimidines. The other two, adenine (A) and guanine (G), are double-ringed structures called purines. These bases form complementary base pairs consisting of one purine and one pyrimidine, with adenine pairing with thymine, and cytosine with guanine. Each base pair is held together by hydrogen bonding. A and T share two hydrogen bonds, C and G share three, and both pairings have a similar shape and structure Figure 8.4.13.

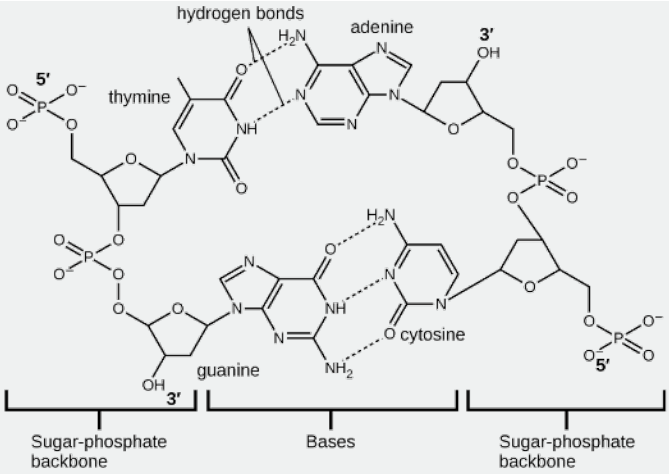


Figure **8.4.13**: The geometries of the base molecules result in maximum hydrogen bonding between adenine and thymine (AT) and between guanine and cytosine (GC), so-called “complementary base pairs.”

The cumulative effect of millions of hydrogen bonds effectively holds the two strands of DNA together. Importantly, the two strands of DNA can relatively easily “unzip” down the middle since hydrogen bonds are relatively weak compared to the covalent bonds that hold the atoms of the individual DNA molecules together. This allows both strands to function as a template for replication.

This page titled 8.4: Intermolecular Forces is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **10.1: Intermolecular Forces** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.5: Types of Solutions

Learning Objectives

By the end of this section, you will be able to:

- Describe the basic properties of solutions and how they form
- Predict whether a given mixture will yield a solution based on molecular properties of its components
- Explain why some solutions either produce or absorb heat when they form

An earlier chapter of this text introduced *solutions*, defined as homogeneous mixtures of two or more substances. Often, one component of a solution is present at a significantly greater concentration, in which case it is called the *solvent*. The other components of the solution present in relatively lesser concentrations are called *solutes*. Sugar is a covalent solid composed of sucrose molecules, $\mathbf{C_{12}H_{22}O_{11}}$. When this compound dissolves in water, its molecules become uniformly distributed among the molecules of water:

$$\mathbf{C_{12}H_{22}O_{11}\,(s) \longrightarrow C_{12}H_{22}O_{11}\,(aq)}$$

The subscript "*aq*" in the equation signifies that the sucrose molecules are solutes and are therefore *individually dispersed* throughout the *aqueous solution* (water is the solvent). Although sucrose molecules are heavier than water molecules, they remain dispersed throughout the solution; gravity does not cause them to "settle out" over time.

Potassium dichromate, $\mathbf{K_2Cr_2O_7}$, is an ionic compound composed of colorless potassium ions, $\mathbf{K^+}$, and orange dichromate ions, $\mathbf{Cr_2O_7^{2-}}$. When a small amount of solid potassium dichromate is added to water, the compound dissolves and dissociates to yield potassium ions and dichromate ions uniformly distributed throughout the mixture (Figure **8.5.1**), as indicated in this equation:

$$\mathbf{K_2Cr_2O_7\,(s) \longrightarrow 2\,K^+\,(aq) + Cr_2O_7^{2-}\,(aq)}$$

As with the mixture of sugar and water, this mixture is also an aqueous solution. Its solutes, potassium and dichromate ions, remain individually dispersed among the solvent (water) molecules.



Figure **8.5.1**: When potassium dichromate ($K_2Cr_2O_7$) is mixed with water, it forms a homogeneous orange solution. (credit: modification of work by Mark Ott)

Link to Learning

Visit this virtual lab to view simulations of the dissolution of common covalent and ionic substances (sugar and salt) in water.

Water is used so often as a solvent that the word solution has come to imply an aqueous solution to many people. However, almost any gas, liquid, or solid can act as a solvent. Many alloys are solid solutions of one metal dissolved in another; for example, US five-cent coins contain nickel dissolved in copper. Air is a gaseous solution, a homogeneous mixture of nitrogen, oxygen, and several other gases. Oxygen (a gas), alcohol (a liquid), and sugar (a solid) all dissolve in water (a liquid) to form liquid solutions. Table **8.5.1** gives examples of several different solutions and the phases of the solutes and solvents.

Table **8.5.1**: Different Types of Solutions

Solution	Solute	Solvent
air	$O_2(g)$	$N_2(g)$
soft drinks[1]	$CO_2(g)$	$H_2O(l)$
hydrogen in palladium	$H_2(g)$	$Pd(s)$
rubbing alcohol	$H_2O(l)$	$C_3H_8O(l)$ (2-propanol)
saltwater	$NaCl(s)$	$H_2O(l)$
brass	$Zn(s)$	$Cu(s)$

Solutions exhibit these defining traits:

- They are homogeneous; after a solution is mixed, it has the same composition at all points throughout (its composition is uniform).
- The physical state of a solution—solid, liquid, or gas—is typically the same as that of the solvent, as demonstrated by the examples in Table **8.5.1**.
- The components of a solution are dispersed on a molecular scale; they consist of a mixture of separated solute particles (molecules, atoms, and/or ions) each closely surrounded by solvent species.
- The dissolved solute in a solution will not settle out or separate from the solvent.
- The composition of a solution, or the concentrations of its components, can be varied continuously (within limits determined by the *solubility* of the components, discussed in detail later in this chapter).

8.5.1: The Formation of Solutions

The formation of a solution is an example of a spontaneous process, a process that occurs under specified conditions without the requirement of energy from some external source. Sometimes a mixture is stirred to speed up the dissolution process, but this is not necessary; a homogeneous solution will form eventually. The topic of spontaneity is critically important to the study of chemical thermodynamics and is treated more thoroughly in a later chapter of this text. For purposes of this chapter's discussion, it will suffice to consider two criteria that *favor*, but do not guarantee, the spontaneous formation of a solution:

1. a decrease in the internal energy of the system (an exothermic change, as discussed in the previous chapter on thermochemistry)
2. an increased dispersal of matter in the system (which indicates an increase in the *entropy* of the system, as you will learn about in the later chapter on thermodynamics)

In the process of dissolution, an internal energy change often, but not always, occurs as heat is absorbed or evolved. An increase in matter dispersal always results when a solution forms from the uniform distribution of solute molecules throughout a solvent.

When the strengths of the intermolecular forces of attraction between solute and solvent species in a solution are no different than those present in the separated components, the solution is formed with no accompanying energy change. Such a solution is called an ideal solution. A mixture of ideal gases (or gases such as helium and argon, which closely approach ideal behavior) is an example of an ideal solution, since the entities comprising these gases experience no significant intermolecular attractions.

When containers of helium and argon are connected, the gases spontaneously mix due to diffusion and form a solution (Figure **8.5.2**). The formation of this solution clearly involves an increase in matter dispersal, since the helium and argon atoms occupy a volume twice as large as that which each occupied before mixing.

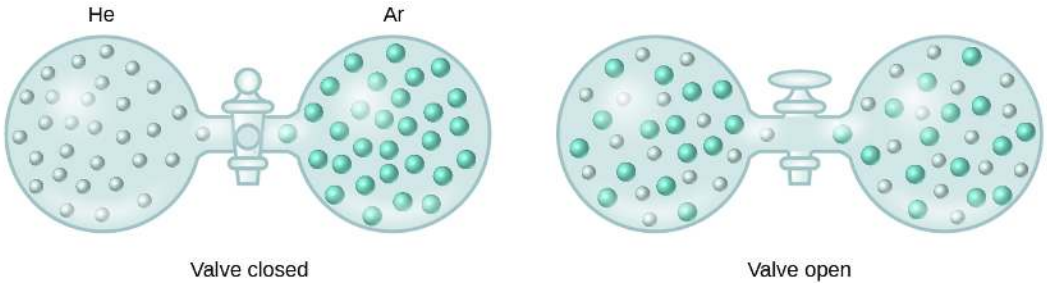


Figure **8.5.2**: Samples of helium and argon spontaneously mix to give a solution.

Ideal solutions may also form when structurally similar liquids are mixed. For example, mixtures of the alcohols methanol (CH_3OH) and ethanol (C_2H_5OH) form ideal solutions, as do mixtures of the hydrocarbons pentane, C_5H_{12}, and hexane, C_6H_{14}. Placing methanol and ethanol, or pentane and hexane, in the bulbs shown in Figure **8.5.2**: will result in the same diffusion and subsequent mixing of these liquids as is observed for the He and Ar gases (although at a much slower rate), yielding solutions with no significant change in energy. Unlike a mixture of gases, however, the components of these liquid-liquid solutions do, indeed, experience intermolecular attractive forces. But since the molecules of the two substances being mixed are structurally very similar, the intermolecular attractive forces between like and unlike molecules are essentially the same, and the dissolution process, therefore, does not entail any appreciable increase or decrease in energy. These examples illustrate how increased matter dispersal alone can provide the driving force required to cause the spontaneous formation of a solution. In some cases, however, the relative magnitudes of intermolecular forces of attraction between solute and solvent species may prevent dissolution.

Three types of intermolecular attractive forces are relevant to the dissolution process: solute-solute, solvent-solvent, and solute-solvent. As illustrated in Figure **8.5.3**: , the formation of a solution may be viewed as a stepwise process in which energy is consumed to overcome solute-solute and solvent-solvent attractions (endothermic processes) and released when solute-solvent attractions are established (an exothermic process referred to as solvation). The relative magnitudes of the energy changes associated with these stepwise processes determine whether the dissolution process overall will release or absorb energy. In some cases, solutions do not form because the energy required to separate solute and solvent species is so much greater than the energy released by solvation.

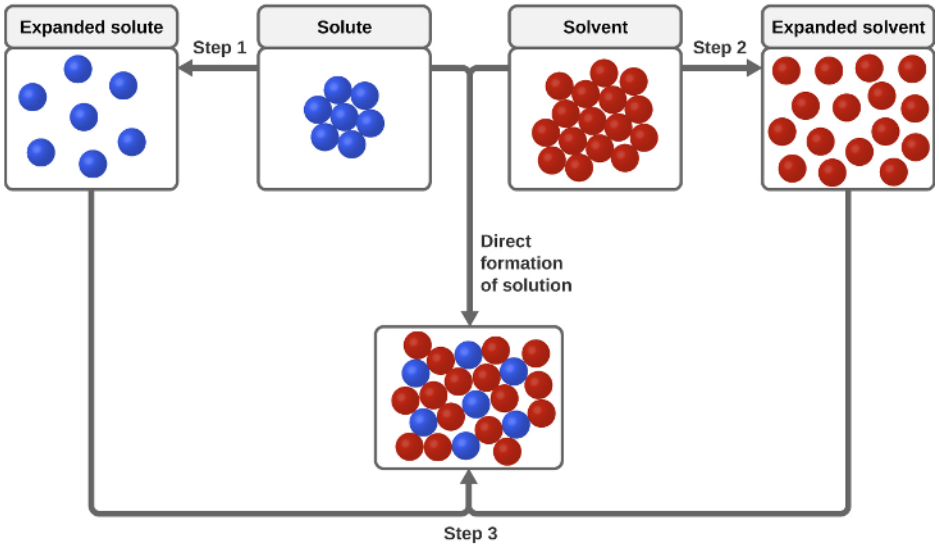


Figure **8.5.3**: This schematic representation of dissolution shows a stepwise process involving the endothermic separation of solute and solvent species (Steps 1 and 2) and exothermic solvation (Step 3).

Consider the example of an ionic compound dissolving in water. Formation of the solution requires the electrostatic forces between the cations and anions of the compound (solute–solute) be overcome completely as attractive forces are established between these ions and water molecules (solute–solvent). Hydrogen bonding between a relatively small fraction of the water molecules must also be overcome to accommodate any dissolved solute. If the solute's electrostatic forces are significantly greater than the solvation

forces, the dissolution process is significantly endothermic and the compound may not dissolve to an appreciable extent. Calcium carbonate, the major component of coral reefs, is one example of such an “insoluble” ionic compound. On the other hand, if the solvation forces are much stronger than the compound’s electrostatic forces, the dissolution is significantly exothermic and the compound may be highly soluble. common example of this type of ionic compound is sodium hydroxide, commonly known as lye.

As noted at the beginning of this module, spontaneous solution formation is favored, but not guaranteed, by exothermic dissolution processes. While many soluble compounds do, indeed, dissolve with the release of heat, some dissolve endothermically. Ammonium nitrate (NH_4NO_3) is one such example and is used to make instant cold packs, like the one pictured in Figure **8.5.4**, which are used for treating injuries. A thin-walled plastic bag of water is sealed inside a larger bag with solid NH_4NO_3. When the smaller bag is broken, a solution of NH_4NO_3 forms, absorbing heat from the surroundings (the injured area to which the pack is applied) and providing a cold compress that decreases swelling. Endothermic dissolutions such as this one require a greater energy input to separate the solute species than is recovered when the solutes are solvated, but they are spontaneous nonetheless due to the increase in disorder that accompanies formation of the solution.



Figure **8.5.4**: An instant cold pack gets cold when certain salts, such as ammonium nitrate, dissolve in water—an endothermic process.

Link to Learning

Watch this brief video illustrating endothermic and exothermic dissolution processes.

8.5.2: Footnotes

- 1If bubbles of gas are observed within the liquid, the mixture is not homogeneous and, thus, not a solution.

This page titled 8.5: Types of Solutions is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **11.1: The Dissolution Process** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.6: Electrolytes

Learning Objectives

By the end of this section, you will be able to:

- Define and give examples of electrolytes
- Distinguish between the physical and chemical changes that accompany dissolution of ionic and covalent electrolytes
- Relate electrolyte strength to solute-solvent attractive forces

When some substances are dissolved in water, they undergo either a physical or a chemical change that yields ions in solution. These substances constitute an important class of compounds called electrolytes. Substances that do not yield ions when dissolved are called nonelectrolytes. If the physical or chemical process that generates the ions is essentially 100% efficient (all of the dissolved compound yields ions), then the substance is known as a strong electrolyte. If only a relatively small fraction of the dissolved substance undergoes the ion-producing process, it is called a weak electrolyte.

Substances may be identified as strong, weak, or nonelectrolytes by measuring the electrical conductance of an aqueous solution containing the substance. To conduct electricity, a substance must contain freely mobile, charged species. Most familiar is the conduction of electricity through metallic wires, in which case the mobile, charged entities are electrons. Solutions may also conduct electricity if they contain dissolved ions, with conductivity increasing as ion concentration increases. Applying a voltage to electrodes immersed in a solution permits assessment of the relative concentration of dissolved ions, either quantitatively, by measuring the electrical current flow, or qualitatively, by observing the brightness of a light bulb included in the circuit (Figure **8.6.1**).

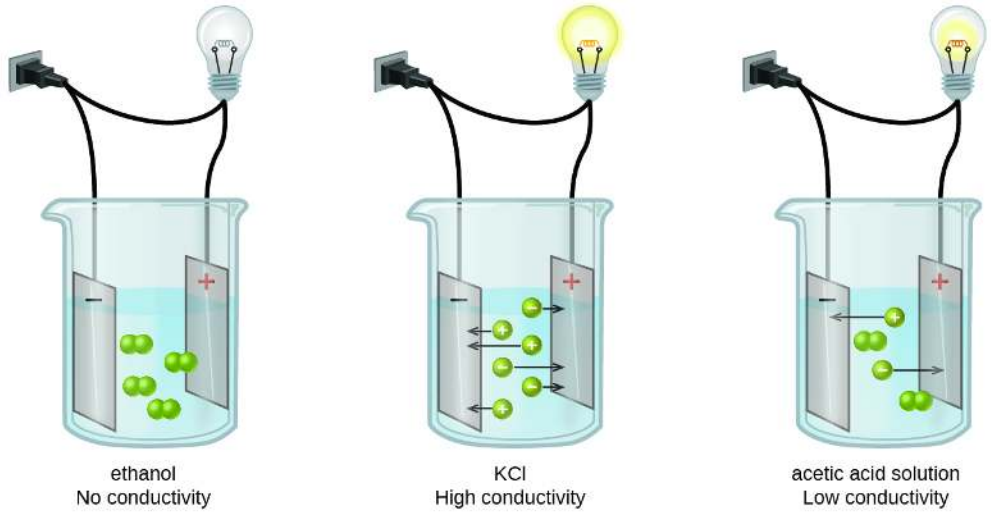


Figure **8.6.1**: Solutions of nonelectrolytes such as ethanol do not contain dissolved ions and cannot conduct electricity. Solutions of electrolytes contain ions that permit the passage of electricity. The conductivity of an electrolyte solution is related to the strength of the electrolyte.

8.6.1: Ionic Electrolytes

Water and other polar molecules are attracted to ions, as shown in Figure **8.6.2**. The electrostatic attraction between an ion and a molecule with a dipole is called an ion-dipole attraction. These attractions play an important role in the dissolution of ionic compounds in water.

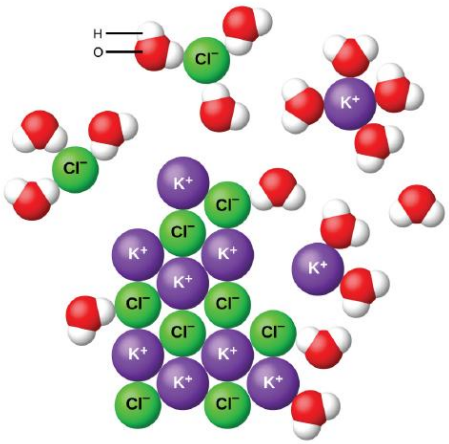


Figure 8.6.2: As potassium chloride (KCl) dissolves in water, the ions are hydrated. The polar water molecules are attracted by the charges on the K^+ and Cl^- ions. Water molecules in front of and behind the ions are not shown.

When ionic compounds dissolve in water, the ions in the solid separate and disperse uniformly throughout the solution because water molecules surround and solvate the ions, reducing the strong electrostatic forces between them. This process represents a physical change known as dissociation. Under most conditions, ionic compounds will dissociate nearly completely when dissolved, and so they are classified as strong electrolytes. Even sparingly, soluble ionic compounds are strong electrolytes, since the small amount that does dissolve will dissociate completely.

Consider what happens at the microscopic level when solid KCl is added to water. Ion-dipole forces attract the positive (hydrogen) end of the polar water molecules to the negative chloride ions at the surface of the solid, and they attract the negative (oxygen) ends to the positive potassium ions. The water molecules surround individual K^+ and Cl^- ions, reducing the strong interionic forces that bind the ions together and letting them move off into solution as solvated ions, as Figure 8.6.2 shows. Overcoming the electrostatic attraction permits the independent motion of each hydrated ion in a dilute solution as the ions transition from fixed positions in the undissolved compound to widely dispersed, solvated ions in solution.

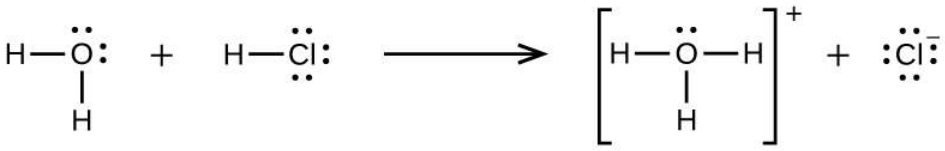
8.6.2: Covalent Electrolytes

Pure water is an extremely poor conductor of electricity because it is only very slightly ionized—only about two out of every 1 billion molecules ionize at 25 °C. Water ionizes when one molecule of water gives up a proton (H^+ ion) to another molecule of water, yielding hydronium and hydroxide ions.

$$\mathbf{H_2O\,(l) + H_2O\,(l) \rightleftharpoons H_3O^+\,(aq) + OH^-\,(aq)}$$

In some cases, solutions prepared from covalent compounds conduct electricity because the solute molecules react chemically with the solvent to produce ions. For example, pure hydrogen chloride is a gas consisting of covalent HCl molecules. This gas contains no ions. However, an aqueous solution of HCl is a very good conductor, indicating that an appreciable concentration of ions exists within the solution.

Because HCl is an *acid*, its molecules react with water, transferring H^+ ions to form hydronium ions (H_3O^+) and chloride ions (Cl^-):



This reaction is essentially 100% complete for HCl (i.e., it is a *strong acid* and, consequently, a strong electrolyte). Likewise, weak acids and bases that only react partially generate relatively low concentrations of ions when dissolved in water and are classified as weak electrolytes. The reader may wish to review the discussion of strong and weak acids provided in the earlier chapter of this text on reaction classes and stoichiometry.

This page titled 8.6: Electrolytes is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **11.2: Electrolytes** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.7: Concentration

Learning Objectives

By the end of this section, you will be able to:

- Describe the fundamental properties of solutions
- Calculate solution concentrations using molarity
- Perform dilution calculations using the dilution equation

Preceding sections of this chapter focused on the composition of substances: samples of matter that contain only one type of element or compound. However, mixtures—samples of matter containing two or more substances physically combined—are more commonly encountered in nature than are pure substances. Similar to a pure substance, the relative composition of a mixture plays an important role in determining its properties. The relative amount of oxygen in a planet's atmosphere determines its ability to sustain aerobic life. The relative amounts of iron, carbon, nickel, and other elements in steel (a mixture known as an "alloy") determine its physical strength and resistance to corrosion. The relative amount of the active ingredient in a medicine determines its effectiveness in achieving the desired pharmacological effect. The relative amount of sugar in a beverage determines its sweetness (see Figure **8.7.1**). This section will describe one of the most common ways in which the relative compositions of mixtures may be quantified.



Figure **8.7.1**: Sugar is one of many components in the complex mixture known as coffee. The amount of sugar in a given amount of coffee is an important determinant of the beverage's sweetness. (credit: Jane Whitney)

8.7.1: Solutions

Solutions have previously been defined as homogeneous mixtures, meaning that the composition of the mixture (and therefore its properties) is uniform throughout its entire volume. Solutions occur frequently in nature and have also been implemented in many forms of manmade technology. A more thorough treatment of solution properties is provided in the chapter on solutions and colloids, but provided here is an introduction to some of the basic properties of solutions.

The relative amount of a given solution component is known as its **concentration**. Often, though not always, a solution contains one component with a concentration that is significantly greater than that of all other components. This component is called the solvent and may be viewed as the medium in which the other components are dispersed, or **dissolved**. Solutions in which water is the solvent are, of course, very common on our planet. A solution in which water is the solvent is called an **aqueous solution**.

A **solute** is a component of a solution that is typically present at a much lower concentration than the solvent. Solute concentrations are often described with qualitative terms such as **dilute** (of relatively low concentration) and **concentrated** (of relatively high concentration).

Concentrations may be quantitatively assessed using a wide variety of measurement units, each convenient for particular applications. **Molarity** (*M*) is a useful concentration unit for many applications in chemistry. Molarity is defined as the number of moles of solute in exactly 1 liter (1 L) of the solution:

$$M = \frac{\text{mol solute}}{\text{L solution}}$$

Example 8.7.1: Calculating Molar Concentrations

A 355-mL soft drink sample contains 0.133 mol of sucrose (table sugar). What is the molar concentration of sucrose in the beverage?

Solution

Since the molar amount of solute and the volume of solution are both given, the molarity can be calculated using the definition of molarity. Per this definition, the solution volume must be converted from mL to L:

$$M = \frac{\text{mol solute}}{\text{L solution}} = \frac{0.133\,\text{mol}}{355\,\text{mL} \times \frac{1\,\text{L}}{1000\,\text{mL}}} = 0.375M$$

Exercise 8.7.1

A teaspoon of table sugar contains about 0.01 mol sucrose. What is the molarity of sucrose if a teaspoon of sugar has been dissolved in a cup of tea with a volume of 200 mL?

Answer

0.05 *M*

Example 8.7.2: Deriving Moles and Volumes from Molar Concentrations

How much sugar (mol) is contained in a modest sip (~10 mL) of the soft drink from Example **8.7.1**?

Solution

Rearrange the definition of molarity to isolate the quantity sought, moles of sugar, then substitute the value for molarity derived in Example **8.7.1**, 0.375 *M*:

$$\begin{aligned} M &= \frac{\text{mol solute}}{L\text{ solution}} \\ \text{mol solute} &= M \times L\text{ solution} \\ &= 0.375\frac{\text{mol sugar}}{L} \times \left(10\,\text{mL} \times \frac{1\,\text{L}}{1000\,\text{mL}}\right) \\ &= 0.004\,\text{mol sugar} \end{aligned}$$

Exercise 8.7.2

What volume (mL) of the sweetened tea described in Example **8.7.1** contains the same amount of sugar (mol) as 10 mL of the soft drink in this example?

Answer

80 mL

Example 8.7.3: Calculating Molar Concentrations from the Mass of Solute

Distilled white vinegar (Figure **8.7.2**) is a solution of acetic acid, CH_3CO_2H, in water. A 0.500-L vinegar solution contains 25.2 g of acetic acid. What is the concentration of the acetic acid solution in units of molarity?



Figure 8.7.2: Distilled white vinegar is a solution of acetic acid in water.

Solution

As in previous examples, the definition of molarity is the primary equation used to calculate the quantity sought. Since the mass of solute is provided instead of its molar amount, use the solute's molar mass to obtain the amount of solute in moles:

$$M = \frac{\text{mol solute}}{\text{L solution}} = \frac{25.2\,\text{g}\,\text{CH}_3\text{CO}_2\text{H} \times \frac{1\,\text{mol}\,\text{CH}_3\text{CO}_2\text{H}}{60.052\,\text{g}\,\text{CH}_3\text{CO}_2\text{H}}}{0.500\,\text{L solution}} = 0.839\,\text{M}$$

Exercise 8.7.3

Calculate the molarity of 6.52 g of $CoCl_2$ (128.9 g/mol) dissolved in an aqueous solution with a total volume of 75.0 mL.

Answer

0.674 *M*

Example 8.7.4: Determining the Mass of Solute in a Given Volume of Solution

How many grams of NaCl are contained in 0.250 L of a 5.30-*M* solution?

Solution

The volume and molarity of the solution are specified, so the amount (mol) of solute is easily computed as demonstrated in Example 8.7.2:

$$\begin{aligned} M &= \frac{\text{mol solute}}{L\text{ solution}} \\ \text{mol solute} &= M \times L\text{ solution} \\ &= 5.30\frac{\text{mol NaCl}}{\text{L}} \times 0.250L \\ &= 1.325\,\text{mol NaCl} \end{aligned}$$

Finally, this molar amount is used to derive the mass of NaCl:

$$1.325\,\text{mol NaCl} \times \frac{58.44\,\text{g NaCl}}{1\,\text{mol NaCl}} = 77.4\,\text{g NaCl}$$

Exercise 8.7.4

How many grams of $CaCl_2$ (110.98 g/mol) are contained in 250.0 mL of a 0.200-*M* solution of calcium chloride?

Answer

5.55 g $CaCl_2$

When performing calculations stepwise, as in Example **8.7.4**, it is important to refrain from rounding any intermediate calculation results, which can lead to rounding errors in the final result. In Example **8.7.4**, the molar amount of NaCl computed in the first step, 1.325 mol, would be properly rounded to 1.32 mol if it were to be reported; however, although the last digit (5) is not significant, it must be retained as a guard digit in the intermediate calculation. If the guard digit had not been retained, the final calculation for the mass of NaCl would have been 77.1 g, a difference of 0.3 g.

In addition to retaining a guard digit for intermediate calculations, rounding errors may also be avoided by performing computations in a single step (see Example **8.7.5**). This eliminates intermediate steps so that only the final result is rounded.

✔ Example 8.7.5: Determining the Volume of Solution Containing a Given Mass of Solute

In Example **8.7.3**, the concentration of acetic acid in white vinegar was determined to be 0.839 *M*. What volume of vinegar contains 75.6 g of acetic acid?

Solution

First, use the molar mass to calculate moles of acetic acid from the given mass:

$$\text{g solute} \times \frac{\text{mol solute}}{\text{g solute}} = \text{mol solute}$$

Then, use the molarity of the solution to calculate the volume of solution containing this molar amount of solute:

$$\text{mol solute} \times \frac{\text{L solution}}{\text{mol solute}} = \text{L solution}$$

Combining these two steps into one yields:

$$\text{g solute} \times \left(\frac{\text{mol solute}}{\text{g solute}}\right) \times \left(\frac{\text{L solution}}{\text{mol solute}}\right) = \text{L solution}$$

$$75.6\,\text{g}\,CH_3CO_2H \left(\frac{\text{mol}\,CH_3CO_2H}{60.05\,\text{g}}\right) \left(\frac{\text{L solution}}{0.839\,\text{mol CH 3}\,CO_2H}\right) = 1.50\,\text{L solution}$$

? Exercise 8.7.5

What volume of a 1.50-*M* KBr solution contains 66.0 g **KBr**?

Answer

0.370 L

8.7.2: Dilution of Solutions

Dilution is the process whereby the concentration of a solution is lessened by the addition of solvent. For example, a glass of iced tea becomes increasingly diluted as the ice melts. The water from the melting ice increases the volume of the solvent (water) and the overall volume of the solution (iced tea), thereby reducing the relative concentrations of the solutes that give the beverage its taste (Figure **8.7.3**).

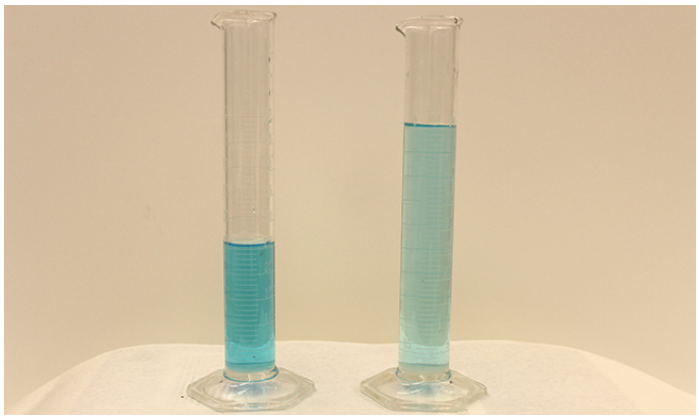


Figure **8.7.3**: Both solutions contain the same mass of copper nitrate. The solution on the right is more dilute because the copper nitrate is dissolved in more solvent. (credit: Mark Ott)

Dilution is also a common means of preparing solutions of a desired concentration. By adding solvent to a measured portion of a more concentrated *stock solution*, a solution of lesser concentration may be prepared. For example, commercial pesticides are typically sold as solutions in which the active ingredients are far more concentrated than is appropriate for their application. Before they can be used on crops, the pesticides must be diluted. This is also a very common practice for the preparation of a number of common laboratory reagents.

A simple mathematical relationship can be used to relate the volumes and concentrations of a solution before and after the dilution process. According to the definition of molarity, the number of moles of solute in a solution (n) is equal to the product of the solution's molarity (M) and its volume in liters (L):

$$n = ML$$

Expressions like these may be written for a solution before and after it is diluted:

$$n_1 = M_1L_1$$
$$n_2 = M_2L_2$$

where the subscripts "1" and "2" refer to the solution before and after the dilution, respectively. Since the dilution process *does not change the amount of solute in the solution*, $n_1 = n_2$. Thus, these two equations may be set equal to one another:

$$M_1L_1 = M_2L_2$$

This relation is commonly referred to as the dilution equation. Although this equation uses molarity as the unit of concentration and liters as the unit of volume, other units of concentration and volume may be used as long as the units properly cancel per the factor-label method. Reflecting this versatility, the dilution equation is often written in the more general form:

$$C_1V_1 = C_2V_2$$

where \(C\) and \(V\) are concentration and volume, respectively.

Link to Learning

Use the simulation to explore the relations between solute amount, solution volume, and concentration and to confirm the dilution equation.

Example 8.7.6: Determining the Concentration of a Diluted Solution

If 0.850 L of a 5.00-*M* solution of copper nitrate, $Cu(NO_3)_2$, is diluted to a volume of 1.80 L by the addition of water, what is the molarity of the diluted solution?

Solution

The stock concentration, C_1, and volume, V_1, are provided as well as the volume of the diluted solution, V_2. Rearrange the dilution equation to isolate the unknown property, the concentration of the diluted solution, C_2:

$$C_1V_1 = C_2V_2$$

$$C_2 = \frac{C_1V_1}{V_2}$$

Since the stock solution is being diluted by more than two-fold (volume is increased from 0.85 L to 1.80 L), the diluted solution's concentration is expected to be less than one-half 5 *M*. This ballpark estimate will be compared to the calculated result to check for any gross errors in computation (for example, such as an improper substitution of the given quantities). Substituting the given values for the terms on the right side of this equation yields:

$$C_2 = \frac{0.850L \times 5.00\frac{mol}{L}}{1.80L} = 2.36M$$

This result compares well to our ballpark estimate (it's a bit less than one-half the stock concentration, 5 *M*).

? Exercise 8.7.6

What is the concentration of the solution that results from diluting 25.0 mL of a 2.04-*M* solution of CH_3OH to 500.0 mL?

Answer

0.102 *M* CH_3OH

✓ Example 8.7.7: Volume of a Diluted Solution

What volume of 0.12 *M* HBr can be prepared from 11 mL (0.011 L) of 0.45 *M* HBr?

Solution

Provided are the volume and concentration of a stock solution, V_1 and C_1, and the concentration of the resultant diluted solution, C_2. Find the volume of the diluted solution, V_2 by rearranging the dilution equation to isolate V_2:

$$C_1V_1 = C_2V_2$$

$$V_2 = \frac{C_1V_1}{C_2}$$

Since the diluted concentration (0.12 *M*) is slightly more than one-fourth the original concentration (0.45 *M*), the volume of the diluted solution is expected to be roughly four times the original volume, or around 44 mL. Substituting the given values and solving for the unknown volume yields:

$$V_2 = \frac{(0.45\,\text{M})(0.011\,\text{L})}{(0.12\,\text{M})}$$

$$= 0.041L$$

The volume of the 0.12-*M* solution is 0.041 L (41 mL). The result is reasonable and compares well with the rough estimate.

? Exercise 8.7.7

A laboratory experiment calls for 0.125 *M* HNO_3. What volume of 0.125 *M* HNO_3 can be prepared from 0.250 L of 1.88 *M* HNO_3?

Answer

3.76 L

✓ Example 8.7.8: Volume of a Concentrated Solution Needed for Dilution

What volume of 1.59 *M* KOH is required to prepare 5.00 L of 0.100 *M* KOH?

Solution

Given are the concentration of a stock solution, C_1, and the volume and concentration of the resultant diluted solution, V_2 and C_2. Find the volume of the stock solution, V_1 by rearranging the dilution equation to isolate V_1:

$$C_1V_1 = C_2V_2$$

$$V_1 = \frac{C_2V_2}{C_1}$$

Since the concentration of the diluted solution 0.100 *M* is roughly one-sixteenth that of the stock solution (1.59 *M*), the volume of the stock solution is expected to be about one-sixteenth that of the diluted solution, or around 0.3 liters. Substituting the given values and solving for the unknown volume yields:

$$V_1 = \frac{(0.100\,\text{M})(5.00\,\text{L})}{1.59\,\text{M}}$$

$$= 0.314\,\text{L}$$

Thus, 0.314 L of the 1.59-*M* solution is needed to prepare the desired solution. This result is consistent with the rough estimate.

? Exercise 8.7.8

What volume of a 0.575-*M* solution of glucose ($\mathbf{C_6H_{12}O_6}$) can be prepared from 50.00 mL of a 3.00-*M* glucose solution?

Answer

0.261 L

This page titled 8.7: Concentration is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **3.3: Molarity** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.7.1: Other Units for Solution Concentrations

Learning Objectives

By the end of this section, you will be able to:

- Define the concentration units of mass percentage, volume percentage, mass-volume percentage, parts-per-million (ppm), and parts-per-billion (ppb)
- Perform computations relating a solution's concentration and its components' volumes and/or masses using these units

The previous section introduced molarity, a very useful measurement unit for evaluating the concentration of solutions. However, molarity is only one measure of concentration. This section will describe some other units of concentration that are commonly used in various applications, either for convenience or by convention.

8.7.1.1: Mass Percentage

Earlier in this chapter, percent composition was introduced as a measure of the relative amount of a given element in a compound. Percentages are also commonly used to express the composition of mixtures, including solutions. The mass percentage of a solution component is defined as the ratio of the component's mass to the solution's mass, expressed as a percentage:

$$\text{mass percentage} = \frac{\text{mass of component}}{\text{mass of solution}} \times 100\%$$

Mass percentage is also referred to by similar names such as *percent mass*, *percent weight*, *weight/weight percent*, and other variations on this theme. The most common symbol for mass percentage is simply the percent sign, %, although more detailed symbols are often used including %mass, %weight, and (w/w)%. Use of these more detailed symbols can prevent confusion of mass percentages with other types of percentages, such as volume percentages (to be discussed later in this section).

Mass percentages are popular concentration units for consumer products. The label of a typical liquid bleach bottle (Figure 8.7.1.1) cites the concentration of its active ingredient, sodium hypochlorite (NaOCl), as being 7.4%. A 100.0-g sample of bleach would therefore contain 7.4 g of NaOCl.



Figure 8.7.1.1: Liquid bleach is an aqueous solution of sodium hypochlorite (NaOCl). This brand has a concentration of 7.4% NaOCl by mass.

Example 8.7.1.1: Calculation of Percent by Mass

A 5.0-g sample of spinal fluid contains 3.75 mg (0.00375 g) of glucose. What is the percent by mass of glucose in spinal fluid?

Solution

The spinal fluid sample contains roughly 4 mg of glucose in 5000 mg of fluid, so the mass fraction of glucose should be a bit less than one part in 1000, or about 0.1%. Substituting the given masses into the equation defining mass percentage yields:

$$\%\ \text{glucose} = \frac{3.75\ \text{mg glucose} \times \frac{1\ \text{g}}{1000\ \text{mg}}}{5.0\ \text{g spinal fluid}} = 0.075\%$$

The computed mass percentage agrees with our rough estimate (it's a bit less than 0.1%).

Note that while any mass unit may be used to compute a mass percentage (mg, g, kg, oz, and so on), the same unit must be used for both the solute and the solution so that the mass units cancel, yielding a dimensionless ratio. In this case, the solute mass unit in the numerator was converted from mg to g to match the units in the denominator. Alternatively, the spinal fluid mass unit in the denominator could have been converted from g to mg instead. As long as identical mass units are used for both solute and solution, the computed mass percentage will be correct.

? Exercise 8.7.1.1

A bottle of a tile cleanser contains 135 g of HCl and 775 g of water. What is the percent by mass of HCl in this cleanser?

Answer

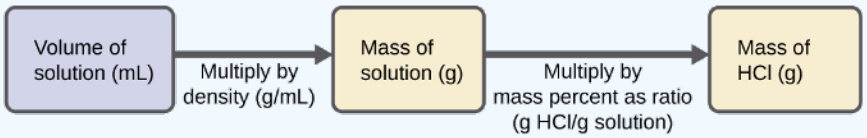
14.8%

✓ Example 8.7.1.2: Calculations using Mass Percentage

"Concentrated" hydrochloric acid is an aqueous solution of 37.2% HCl that is commonly used as a laboratory reagent. The density of this solution is 1.19 g/mL. What mass of HCl is contained in 0.500 L of this solution?

Solution

The HCl concentration is near 40%, so a 100-g portion of this solution would contain about 40 g of HCl. Since the solution density isn't greatly different from that of water (1 g/mL), a reasonable estimate of the HCl mass in 500 g (0.5 L) of the solution is about five times greater than that in a 100 g portion, or 5 40 = 200 g. In order to derive the mass of solute in a solution from its mass percentage, the mass of the solution must be known. Using the solution density given, convert the solution's volume to mass, and then use the given mass percentage to calculate the solute mass. This mathematical approach is outlined in this flowchart:



For proper unit cancellation, the 0.500-L volume is converted into 500 mL, and the mass percentage is expressed as a ratio, 37.2 g HCl/g solution:

$$500 mL\ \text{solution}\left(\frac{1.19\ \text{g solution}}{mL\ \text{solution}}\right)\left(\frac{37.2\ \text{g HCl}}{100\ \text{g solution}}\right) = 221\ \text{g HCl}$$

This mass of HCl is consistent with our rough estimate of approximately 200 g.

? Exercise 8.7.1.2

What volume of concentrated HCl solution contains 125 g of HCl?

Answer

282 mL

8.7.1.2: Volume Percentage

Liquid volumes over a wide range of magnitudes are conveniently measured using common and relatively inexpensive laboratory equipment. The concentration of a solution formed by dissolving a liquid solute in a liquid solvent is therefore often expressed as a volume percentage, %vol or (v/v)%:

$$\text{volume percentage} = \frac{\text{volume solute}}{\text{volume solution}} \times 100\%$$

Example 8.7.1.3: Calculations using Volume Percentage

Rubbing alcohol (isopropanol) is usually sold as a 70%vol aqueous solution. If the density of isopropyl alcohol is 0.785 g/mL, how many grams of isopropyl alcohol are present in a 355 mL bottle of rubbing alcohol?

Solution

Per the definition of volume percentage, the isopropanol volume is 70% of the total solution volume. Multiplying the isopropanol volume by its density yields the requested mass:

\text is only supported in math mode

Exercise 8.7.1.3

Wine is approximately 12% ethanol (CH_3CH_2OH) by volume. Ethanol has a molar mass of 46.06 g/mol and a density 0.789 g/mL. How many moles of ethanol are present in a 750-mL bottle of wine?

Answer

1.5 mol ethanol

8.7.1.3: Mass-Volume Percentage

“Mixed” percentage units, derived from the mass of solute and the volume of solution, are popular for certain biochemical and medical applications. A **mass-volume percent** is a ratio of a solute’s mass to the solution’s volume expressed as a percentage. The specific units used for solute mass and solution volume may vary, depending on the solution. For example, physiological saline solution, used to prepare intravenous fluids, has a concentration of 0.9% mass/volume (m/v), indicating that the composition is 0.9 g of solute per 100 mL of solution. The concentration of glucose in blood (commonly referred to as “blood sugar”) is also typically expressed in terms of a mass-volume ratio. Though not expressed explicitly as a percentage, its concentration is usually given in milligrams of glucose per deciliter (100 mL) of blood (Figure 8.7.1.2).



(a) (b)

Figure 8.7.1.2: “Mixed” mass-volume units are commonly encountered in medical settings. (a) The NaCl concentration of physiological saline is 0.9% (m/v). (b) This device measures glucose levels in a sample of blood. The normal range for glucose concentration in blood (fasting) is around 70–100 mg/dL. (credit a: modification of work by “The National Guard”/Flickr; credit b: modification of work by Biswarup Ganguly)

8.7.1.4: Parts per Million and Parts per Billion

Very low solute concentrations are often expressed using appropriately small units such as parts per million (ppm) or parts per billion (ppb). Like percentage (“part per hundred”) units, ppm and ppb may be defined in terms of masses, volumes, or mixed mass-volume units. There are also ppm and ppb units defined with respect to numbers of atoms and molecules.

The mass-based definitions of ppm and ppb are given here:

$$\text{ppm} = \frac{\text{mass solute}}{\text{mass solution}} \times 10^6 \text{ ppm}$$

$$\text{ppb} = \frac{\text{mass solute}}{\text{mass solution}} \times 10^9 \text{ ppb}$$

Both ppm and ppb are convenient units for reporting the concentrations of pollutants and other trace contaminants in water. Concentrations of these contaminants are typically very low in treated and natural waters, and their levels cannot exceed relatively low concentration thresholds without causing adverse effects on health and wildlife. For example, the EPA has identified the maximum safe level of fluoride ion in tap water to be 4 ppm. Inline water filters are designed to reduce the concentration of fluoride and several other trace-level contaminants in tap water (Figure 8.7.1.3).



(a) (b)

Figure 8.7.1.3: (a) In some areas, trace-level concentrations of contaminants can render unfiltered tap water unsafe for drinking and cooking. (b) Inline water filters reduce the concentration of solutes in tap water. (credit a: modification of work by Jenn Durfey; credit b: modification of work by “vastateparkstaff”/Wikimedia commons)

Example 8.7.1.4: Calculation of Parts per Million and Parts per Billion Concentrations

According to the EPA, when the concentration of lead in tap water reaches 15 ppb, certain remedial actions must be taken. What is this concentration in ppm? At this concentration, what mass of lead (μg) would be contained in a typical glass of water (300 mL)?

Solution

The definitions of the ppm and ppb units may be used to convert the given concentration from ppb to ppm. Comparing these two unit definitions shows that ppm is 1000 times greater than ppb (1 ppm = 10^3 ppb). Thus:

$$15\,\text{ppb} \times \frac{1\,\text{ppm}}{10^3\,\text{ppb}} = 0.015\,\text{ppm}$$

The definition of the ppb unit may be used to calculate the requested mass if the mass of the solution is provided. Since the volume of solution (300 mL) is given, its density must be used to derive the corresponding mass. Assume the density of tap water to be roughly the same as that of pure water (~1.00 g/mL), since the concentrations of any dissolved substances should not be very large. Rearranging the equation defining the ppb unit and substituting the given quantities yields:

$$\text{ppb} = \frac{\text{mass solute}}{\text{mass solution}} \times 10^9\,\text{ppb}$$

$$\text{mass solute} = \frac{\text{ppb} \times \text{mass solution}}{10^9\,\text{ppb}}$$

$$= \frac{15\,\text{ppb} \times 300 mL \times \frac{1.00\,\text{g}}{\text{mL}}}{10^9\,\text{ppb}} = 4.5 \times 10^{-6}\,\text{g}$$

Finally, convert this mass to the requested unit of micrograms:

$$4.5 \times 10^{-6}\,\text{g} \times \frac{1\,\mu g}{10^{-6}\,\text{g}} = 4.5\,\mu g$$

Exercise 8.7.1.4

A 50.0-g sample of industrial wastewater was determined to contain 0.48 mg of mercury. Express the mercury concentration of the wastewater in ppm and ppb units.

Answer

9.6 ppm, 9600 ppb

This page titled 8.7.1: Other Units for Solution Concentrations is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **3.4: Other Units for Solution Concentrations** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.8: Osmosis, Diffusion and Dialysis

Learning Objectives

By the end of this section, you will be able to:

- Express concentrations of solution components using mole fraction and molality
- Describe the effect of solute concentration on various solution properties (vapor pressure, boiling point, freezing point, and osmotic pressure)
- Perform calculations using the mathematical equations that describe these various colligative effects
- Describe the process of distillation and its practical applications
- Explain the process of osmosis and describe how it is applied industrially and in nature

The properties of a solution are different from those of either the pure solute(s) or solvent. Many solution properties are dependent upon the chemical identity of the solute. Compared to pure water, a solution of hydrogen chloride is more acidic, a solution of ammonia is more basic, a solution of sodium chloride is more dense, and a solution of sucrose is more viscous. There are a few solution properties, however, that depend *only* upon the total concentration of solute species, regardless of their identities. These **colligative properties** include vapor pressure lowering, boiling point elevation, freezing point depression, and osmotic pressure. This small set of properties is of central importance to many natural phenomena and technological applications, as will be described in this module.

8.8.1: Mole Fraction and Molality

Several units commonly used to express the concentrations of solution components were introduced in an earlier chapter of this text, each providing certain benefits for use in different applications. For example, molarity (*M*) is a convenient unit for use in stoichiometric calculations, since it is defined in terms of the molar amounts of solute species:

$$M = \frac{\text{mol solute}}{\text{L solution}}$$

Because solution volumes vary with temperature, molar concentrations will likewise vary. When expressed as molarity, the concentration of a solution with identical numbers of solute and solvent species will be different at different temperatures, due to the contraction/expansion of the solution. More appropriate for calculations involving many colligative properties are mole-based concentration units whose values are not dependent on temperature. Two such units are *mole fraction* (introduced in the previous chapter on gases) and *molality*.

The mole fraction, X, of a component is the ratio of its molar amount to the total number of moles of all solution components:

$$X_A = \frac{molA}{\text{total mol of all components}}$$

By this definition, the sum of mole fractions for all solution components (the solvent and all solutes) is equal to one.

Molality is a concentration unit defined as the ratio of the numbers of moles of solute to the mass of the solvent in kilograms:

$$m = \frac{\text{mol solute}}{kg \text{ solvent}}$$

Since these units are computed using only masses and molar amounts, they do not vary with temperature and, thus, are better suited for applications requiring temperature-independent concentrations, including several colligative properties, as will be described in this chapter module.

Example 8.8.1: Calculating Mole Fraction and Molality

The antifreeze in most automobile radiators is a mixture of equal volumes of ethylene glycol and water, with minor amounts of other additives that prevent corrosion. What are the (a) mole fraction and (b) molality of ethylene glycol, $C_2H_4(OH)_2$, in a

solution prepared from 2.22 \times 10^{3} g of ethylene glycol and 2.00 \times 10^{3} g of water (approximately 2 L of glycol and 2 L of water)?

Solution

(a) The mole fraction of ethylene glycol may be computed by first deriving molar amounts of both solution components and then substituting these amounts into the definition of mole fraction.

$$mol C_2H_4(OH)_2 = 2.22 \times 10^3 g \times \frac{1 mol C_2H_4(OH)_2}{62.07 g C_2H_4(OH)_2} = 35.8 mol C_2H_4(OH)_2$$

$$mol H_2O = 2.00 \times 10^3 g \times \frac{1 mol H_2O}{18.02 g H_2O} = 111 mol H_2O$$

$$X_{\text{ethylene glycol}} = \frac{35.8 mol C_2H_4(OH)_2}{(35.8 + 111)\ \text{mol total}} = 0.244$$

Notice that mole fraction is a dimensionless property, being the ratio of properties with identical units (moles).

(b) Derive moles of solute and mass of solvent (in kg).

First, use the given mass of ethylene glycol and its molar mass to find the moles of solute:

$$2.22 \times 10^3 g C_2H_4(OH)_2 \left(\frac{mol C_2H_2(OH)_2}{62.07 g}\right) = 35.8 mol C_2H_4(OH)_2$$

Then, convert the mass of the water from grams to kilograms:

$$2.00 \times 10^3 g H_2O \left(\frac{1 kg}{1000 g}\right) = 2.00 kg H_2O$$

Finally, calculate molality per its definition:

$$\begin{aligned} \text{molality} &= \frac{\text{mol solute}}{\text{kg solvent}} \\ &= \frac{35.8 mol C_2H_4(OH)_2}{2 kg H_2O} \\ &= 17.9 m \end{aligned}$$

? Exercise 8.8.1

What are the mole fraction and molality of a solution that contains 0.850 g of ammonia, NH_3, dissolved in 125 g of water?

Answer

7.14 \times 10^{−3}; 0.399 *m*

✓ Example 8.8.2: Converting Mole Fraction and Molal Concentrations

Calculate the mole fraction of solute and solvent in a 3.0 *m* solution of sodium chloride.

Solution

Converting from one concentration unit to another is accomplished by first comparing the two unit definitions. In this case, both units have the same numerator (moles of solute) but different denominators. The provided molal concentration may be written as:

$$\frac{3.0 mol NaCl}{1 kg H_2O}$$

The numerator for this solution's mole fraction is, therefore, 3.0 mol NaCl. The denominator may be computed by deriving the molar amount of water corresponding to 1.0 kg

$$1.0 kg H_2O \left(\frac{1000 g}{1 kg}\right)\left(\frac{mol H_2O}{18.02 g}\right) = 55 mol H_2O$$

and then substituting these molar amounts into the definition for mole fraction.

$$\begin{aligned} X_{H_2O} &= \frac{mol H_2O}{mol NaCl + mol H_2O} \\ &= \frac{55 mol H_2O}{3.0 mol NaCl + 55 mol H_2O} \\ &= 0.95 \\ &= \frac{mol NaCl}{mol NaCl + mol H H_2O} \\ &= \frac{3.0 mol NaCl}{3.0 mol NaCl + 55 mol H_2O} \\ &= 0.052 \end{aligned}$$

Exercise 8.8.2

The mole fraction of iodine, I_2, dissolved in dichloromethane, CH_2Cl_2, is 0.115. What is the molal concentration, m, of iodine in this solution?

Answer

1.50 m

Example 8.8.3: Molality and Molarity Conversions

Intravenous infusion of a 0.556 M aqueous solution of glucose (density of 1.04 g/mL) is part of some post-operative recovery therapies. What is the molal concentration of glucose in this solution?

Solution

The provided molal concentration may be explicitly written as:

$$M = 0.556 mol \text{ glucose } / 1 L \text{ solution}$$

Consider the definition of molality:

$$m = \text{ mol solute } / kg \text{ solvent}$$

The amount of glucose in 1-L of this solution is 0.556 mol, so the mass of water in this volume of solution is needed.

First, compute the mass of 1.00 L of the solution:

$$(1.0 L \text{ soln })(1.04 g/mL)(1000 mL/1 L)(1 kg/1000 g) = 1.04 kg \text{ soln}$$

This is the mass of both the water and its solute, glucose, and so the mass of glucose must be subtracted. Compute the mass of glucose from its molar amount:

$$(0.556 mol \text{ glucose })(180.2 g/1 mol) = 100.2 g \text{ or } 0.1002 kg$$

Subtracting the mass of glucose yields the mass of water in the solution:

$$1.04 kg \text{ solution } - 0.1002 kg \text{ glucose } = 0.94 kg \text{ water}$$

Finally, the molality of glucose in this solution is computed as:

$$m = \frac{0.556 \text{ mol glucose}}{0.94 \text{ kg water}} = 0.59 \ m$$

? Exercise 8.8.3

Nitric acid, $HNO_3(aq)$, is commercially available as a 33.7 m aqueous solution (density = 1.35 g/mL). What is the molarity of this solution?

Answer

14.6 M

8.8.2: Vapor Pressure Lowering

As described in the chapter on liquids and solids, the equilibrium vapor pressure of a liquid is the pressure exerted by its gaseous phase when vaporization and condensation are occurring at equal rates:

$$\text{liquid} \rightleftharpoons \text{gas}$$

Dissolving a nonvolatile substance in a volatile liquid results in a lowering of the liquid's vapor pressure. This phenomenon can be rationalized by considering the effect of added solute molecules on the liquid's vaporization and condensation processes. To vaporize, solvent molecules must be present at the surface of the solution. The presence of solute decreases the surface area available to solvent molecules and thereby reduces the rate of solvent vaporization. Since the rate of condensation is unaffected by the presence of solute, the net result is that the vaporization-condensation equilibrium is achieved with fewer solvent molecules in the vapor phase (i.e., at a lower vapor pressure) (Figure 8.8.1). While this interpretation is useful, it does not account for several important aspects of the colligative nature of vapor pressure lowering. A more rigorous explanation involves the property of entropy, a topic of discussion in a later text chapter on thermodynamics. For purposes of understanding the lowering of a liquid's vapor pressure, it is adequate to note that the more dispersed nature of matter in a solution, compared to separate solvent and solute phases, serves to effectively stabilize the solvent molecules and hinder their vaporization. A lower vapor pressure results, and a correspondingly higher boiling point as described in the next section of this module.

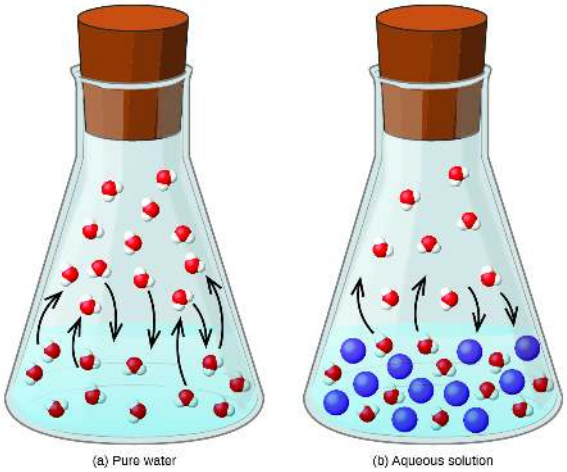


Figure 8.8.1: The presence of nonvolatile solutes lowers the vapor pressure of a solution by impeding the evaporation of solvent molecules.

The relationship between the vapor pressures of solution components and the concentrations of those components is described by **Raoult's law**: *The partial pressure exerted by any component of an ideal solution is equal to the vapor pressure of the pure component multiplied by its mole fraction in the solution.*

$$P_A = X_A P_A^* \tag{8.8.1}$$

where P_A is the partial pressure exerted by component A in the solution, P_A^* is the vapor pressure of pure A, and X_A is the mole fraction of A in the solution.

Recalling that the total pressure of a gaseous mixture is equal to the sum of partial pressures for all its components (Dalton's law of partial pressures), the total vapor pressure exerted by a solution containing *i* components is

$$P_{\text{solution}} = \sum_i P_i = \sum_i X_i P_i^*$$

A nonvolatile substance is one whose vapor pressure is negligible ($P^* \approx 0$), and so the vapor pressure above a solution containing only nonvolatile solutes is due only to the solvent:

$$P_{\text{solution}} = X_{\text{solvent}} P^*_{\text{solvent}}$$

Example 8.8.4: Calculation of a Vapor Pressure

Compute the vapor pressure of an ideal solution containing 92.1 g of glycerin, $C_3H_5(OH)_3$, and 184.4 g of ethanol, C_2H_5OH, at 40 °C. The vapor pressure of pure ethanol is 0.178 atm at 40 °C. Glycerin is essentially nonvolatile at this temperature.

Solution

Since the solvent is the only volatile component of this solution, its vapor pressure may be computed per Raoult's law (Equation 8.8.1) as:

$$P_{\text{solution}} = X_{\text{solvent}} P^*_{\text{solvent}}$$

First, calculate the molar amounts of each solution component using the provided mass data.

$$92.1 g_3 H_5(OH)_3 \times \frac{1 mol C_3 H_5(OH)_3}{92.094 g_5 C_3 H_5(OH)_3} = 1.00 mol C_3 H_5(OH)_3$$

$$184.4 g_2 C_2 H_5 OH \times \frac{1 mol C_2 H_5 OH}{46.069 g_2 C H_5 OH} = 4.000 mol C_2 H_5 OH$$

Next, calculate the mole fraction of the solvent (ethanol) and use Raoult's law to compute the solution's vapor pressure.

$$X_{C_2H_5OH} = \frac{4.000 mol}{(1.00 mol + 4.000 mol)} = 0.800$$

$$P_{\text{solv}} = X_{\text{solv}} P^*_{\text{solv}} = 0.800 \times 0.178 atm = 0.142 atm$$

Exercise 8.8.4

A solution contains 5.00 g of urea, $CO(NH_2)_2$ (a nonvolatile solute) and 0.100 kg of water. If the vapor pressure of pure water at 25 °C is 23.7 torr, what is the vapor pressure of the solution assuming ideal behavior?

Answer

23.4 torr

8.8.3: Distillation of Solutions

Solutions whose components have significantly different vapor pressures may be separated by a selective vaporization process known as distillation. Consider the simple case of a mixture of two volatile liquids, A and B, with A being the more volatile liquid. Raoult's law can be used to show that the vapor above the solution is enriched in component A, that is, the mole fraction of A in the vapor is greater than the mole fraction of A in the liquid (see end-of-chapter Exercise 65). By appropriately heating the mixture, component A may be vaporized, condensed, and collected—effectively separating it from component B.

Distillation is widely applied in both laboratory and industrial settings, being used to refine petroleum, to isolate fermentation products, and to purify water. A typical apparatus for laboratory-scale distillations is shown in Figure 8.8.2.

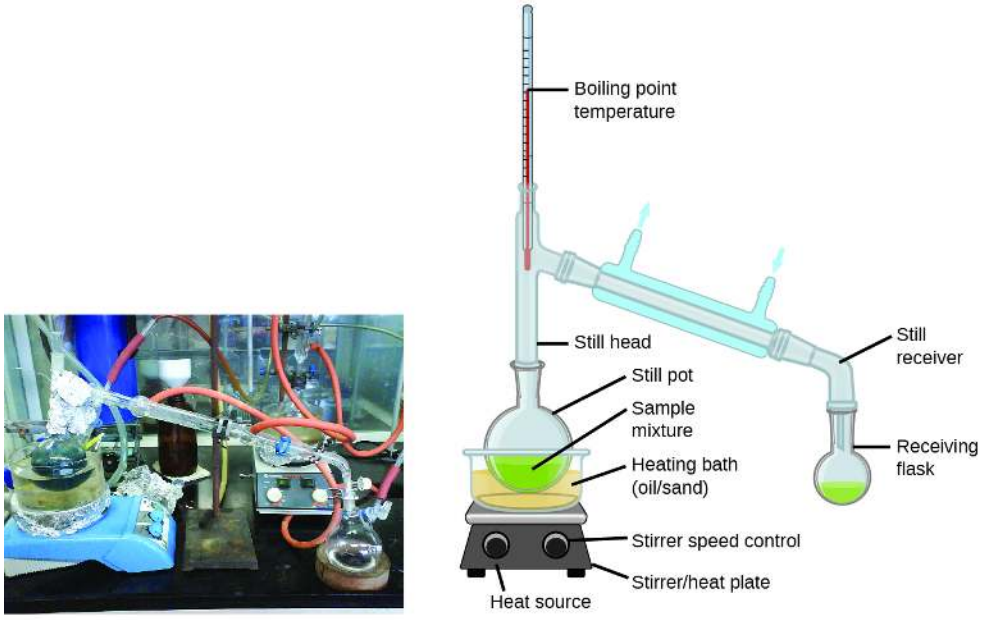


Figure 8.8.2: A typical laboratory distillation unit is shown in (a) a photograph and (b) a schematic diagram of the components. (credit a: modification of work by "Rifleman82"/Wikimedia commons; credit b: modification of work by "Slashme"/Wikimedia Commons)

Oil refineries use large-scale *fractional distillation* to separate the components of crude oil. The crude oil is heated to high temperatures at the base of a tall *fractionating column*, vaporizing many of the components that rise within the column. As vaporized components reach adequately cool zones during their ascent, they condense and are collected. The collected liquids are simpler mixtures of hydrocarbons and other petroleum compounds that are of appropriate composition for various applications (e.g., diesel fuel, kerosene, gasoline), as depicted in Figure 8.8.3.

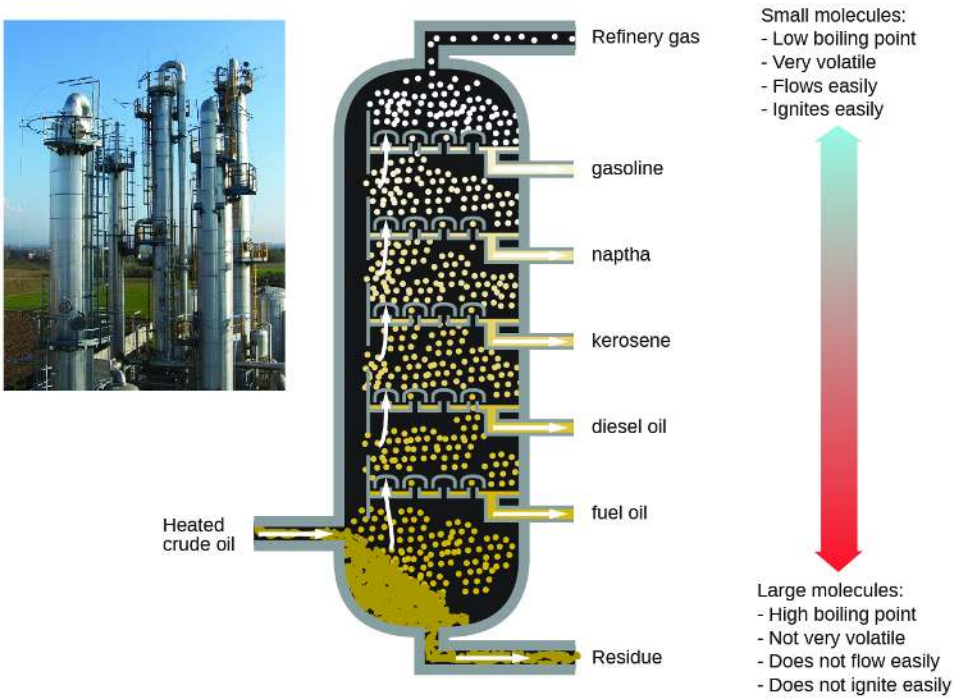


Figure 8.8.3: Crude oil is a complex mixture that is separated by large-scale fractional distillation to isolate various simpler mixtures.

8.8.4: Boiling Point Elevation

As described in the chapter on liquids and solids, the *boiling point* of a liquid is the temperature at which its vapor pressure is equal to ambient atmospheric pressure. Since the vapor pressure of a solution is lowered due to the presence of nonvolatile solutes, it stands to reason that the solution's boiling point will subsequently be increased. Vapor pressure increases with temperature, and so a solution will require a higher temperature than will pure solvent to achieve any given vapor pressure, including one equivalent to that of the surrounding atmosphere. The increase in boiling point observed when nonvolatile solute is dissolved in a solvent, ΔT_b, is called **boiling point elevation** and is directly proportional to the molal concentration of solute species:

$$\Delta T_b = K_b m$$

where K_b is the boiling point elevation constant, or the *ebullioscopic constant* and m is the molal concentration (molality) of all solute species.

Boiling point elevation constants are characteristic properties that depend on the identity of the solvent. Values of K_b for several solvents are listed in Table 8.8.1.

Table 8.8.1: Boiling Point Elevation and Freezing Point Depression Constants for Several Solvents

Solvent	Boiling Point (°C at 1 atm)	K_b (°Cm^{-1})	Freezing Point (°C at 1 atm)	K_f (°Cm^{-1})
water	100.0	0.512	0.0	1.86
hydrogen acetate	118.1	3.07	16.6	3.9
benzene	80.1	2.53	5.5	5.12
chloroform	61.26	3.63	−63.5	4.68
nitrobenzene	210.9	5.24	5.67	8.1

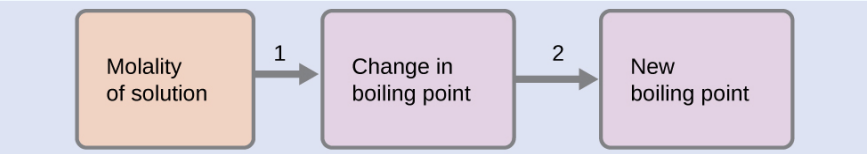
The extent to which the vapor pressure of a solvent is lowered and the boiling point is elevated depends on the total number of solute particles present in a given amount of solvent, not on the mass or size or chemical identities of the particles. A 1 *m* aqueous solution of sucrose (342 g/mol) and a 1 *m* aqueous solution of ethylene glycol (62 g/mol) will exhibit the same boiling point because each solution has one mole of solute particles (molecules) per kilogram of solvent.

Example 8.8.5: Calculating the Boiling Point of a Solution

Assuming ideal solution behavior, what is the boiling point of a 0.33 *m* solution of a nonvolatile solute in benzene?

Solution

Use the equation relating boiling point elevation to solute molality to solve this problem in two steps.



Step 1: Calculate the change in boiling point.

$$\Delta T_b = K_b m = 2.53°C m^{-1} \times 0.33 m = 0.83°C$$

Step 2: Add the boiling point elevation to the pure solvent's boiling point.

$$\text{Boiling temperature } = 80.1°C + 0.83°C = 80.9°C$$

? Exercise 8.8.1

Assuming ideal solution behavior, what is the boiling point of the antifreeze described in Example 8.8.1?

Answer

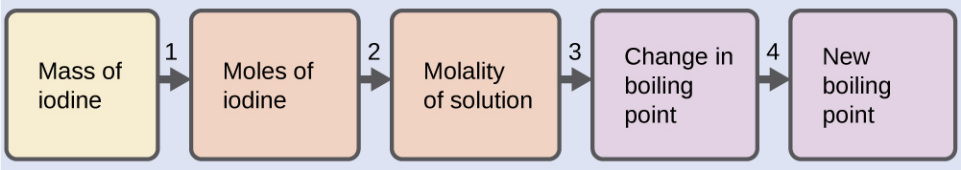
109.2 °C

✓ Example 8.8.6: The Boiling Point of an Iodine Solution

Find the boiling point of a solution of 92.1 g of iodine, I_2, in 800.0 g of chloroform, $CHCl_3$, assuming that the iodine is nonvolatile and that the solution is ideal.

Solution

A four-step approach to solving this problem is outlined below.



Step 1. *Convert from grams to moles of* I_2 *using the molar mass of* I_2 *in the unit conversion factor.*

Result: 0.363 mol

Step 2. *Determine the molality of the solution from the number of moles of solute and the mass of solvent, in kilograms.*

Result: 0.454 *m*

Step 3. *Use the direct proportionality between the change in boiling point and molal concentration to determine how much the boiling point changes.*

Result: 1.65 °C

Step 4. *Determine the new boiling point from the boiling point of the pure solvent and the change.*

Result: 62.91 °C

Check each result as a self-assessment.

? Exercise 8.8.5

What is the boiling point of a solution of 1.0 g of glycerin, $C_3H_5(OH)_3$, in 47.8 g of water? Assume an ideal solution.

Answer

100.12 °C

8.8.5: Freezing Point Depression

Solutions freeze at lower temperatures than pure liquids. This phenomenon is exploited in “de-icing” schemes that use salt (Figure 8.8.4), calcium chloride, or urea to melt ice on roads and sidewalks, and in the use of ethylene glycol as an “antifreeze” in automobile radiators. Seawater freezes at a lower temperature than fresh water, and so the Arctic and Antarctic oceans remain unfrozen even at temperatures below 0 °C (as do the body fluids of fish and other cold-blooded sea animals that live in these oceans).



Figure 8.8.4: Rock salt (NaCl), calcium chloride ($CaCl_2$), or a mixture of the two are used to melt ice. (credit: modification of work by Eddie Welker)

The decrease in freezing point of a dilute solution compared to that of the pure solvent, ΔT_f, is called the **freezing point depression** and is directly proportional to the molal concentration of the solute

$$\Delta T_f = K_f m$$

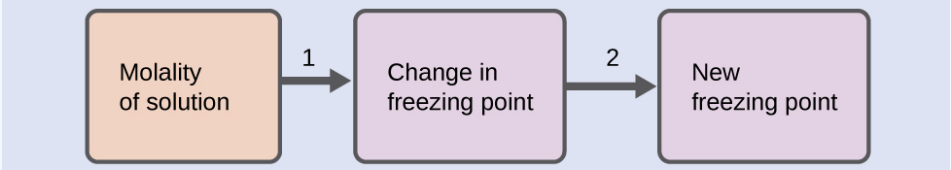
where m is the molal concentration of the solute and K_f is called the freezing point depression constant (or *cryoscopic constant*). Just as for boiling point elevation constants, these are characteristic properties whose values depend on the chemical identity of the solvent. Values of K_f for several solvents are listed in Table 8.8.1.

Example 8.8.7: Calculation of the Freezing Point of a Solution

Assuming ideal solution behavior, what is the freezing point of the 0.33 m solution of a nonvolatile nonelectrolyte solute in benzene described in Example 8.8.2?

Solution

Use the equation relating freezing point depression to solute molality to solve this problem in two steps.



Step 1: Calculate the change in freezing point.

$$\Delta T_f = K_f m = 5.12^\circ C m^{-1} \times 0.33 m = 1.7^\circ C$$

Step 2: Subtract the freezing point change observed from the pure solvent's freezing point.

$$\text{Freezing Temperature } = 5.5^\circ C - 1.7^\circ C = 3.8^\circ C$$

Exercise 8.8.1

Assuming ideal solution behavior, what is the freezing point of a 1.85 m solution of a nonvolatile nonelectrolyte solute in nitrobenzene?

Answer

−9.3 °C

Chemistry in Everyday Life: Colligative Properties and De-Icing

Sodium chloride and its group 2 analogs calcium and magnesium chloride are often used to de-ice roadways and sidewalks, due to the fact that a solution of any one of these salts will have a freezing point lower than 0 °C, the freezing point of pure water. The group 2 metal salts are frequently mixed with the cheaper and more readily available sodium chloride (“rock salt”) for use on roads, since they tend to be somewhat less corrosive than the NaCl, and they provide a larger depression of the freezing point, since they dissociate to yield three particles per formula unit, rather than two particles like the sodium chloride.

Because these ionic compounds tend to hasten the corrosion of metal, they would not be a wise choice to use in antifreeze for the radiator in your car or to de-ice a plane prior to takeoff. For these applications, covalent compounds, such as ethylene or propylene glycol, are often used. The glycols used in radiator fluid not only lower the freezing point of the liquid, but they elevate the boiling point, making the fluid useful in both winter and summer. Heated glycols are often sprayed onto the surface of airplanes prior to takeoff in inclement weather in the winter to remove ice that has already formed and prevent the formation of more ice, which would be particularly dangerous if formed on the control surfaces of the aircraft (Figure 8.8.5).



Figure 8.8.5: Freezing point depression is exploited to remove ice from (a) roadways and (b) the control surfaces of aircraft.

8.8.6: Phase Diagram for a Solution

The colligative effects on vapor pressure, boiling point, and freezing point described in the previous section are conveniently summarized by comparing the phase diagrams for a pure liquid and a solution derived from that liquid (Figure 8.8.6).

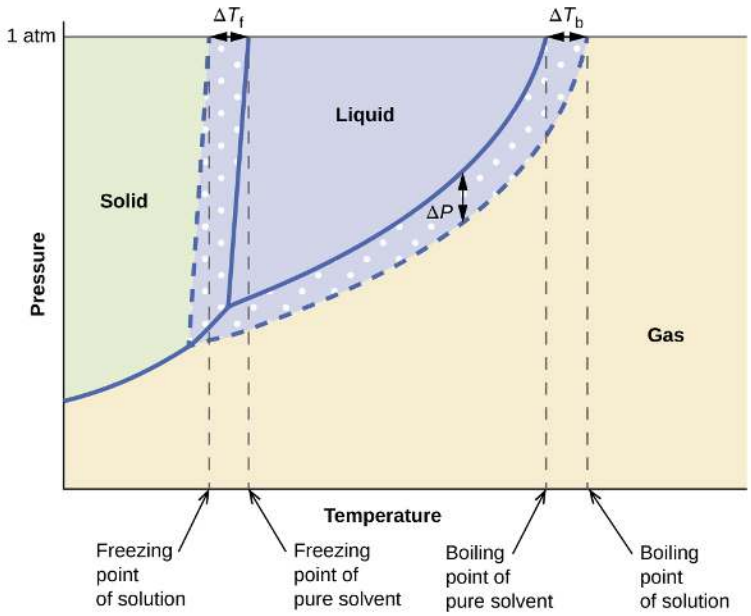


Figure 8.8.6: Phase diagrams for a pure solvent (solid curves) and a solution formed by dissolving nonvolatile solute in the solvent (dashed curves).

The liquid-vapor curve for the solution is located *beneath* the corresponding curve for the solvent, depicting the vapor pressure *lowering*, ΔP, that results from the dissolution of nonvolatile solute. Consequently, at any given pressure, the solution’s boiling

point is observed at a higher temperature than that for the pure solvent, reflecting the boiling point elevation, ΔT_b, associated with the presence of nonvolatile solute. The solid-liquid curve for the solution is displaced left of that for the pure solvent, representing the freezing point depression, ΔT_f, that accompanies solution formation. Finally, notice that the solid-gas curves for the solvent and its solution are identical. This is the case for many solutions comprising liquid solvents and nonvolatile solutes. Just as for vaporization, when a solution of this sort is frozen, it is actually just the *solvent* molecules that undergo the liquid-to-solid transition, forming pure solid solvent that excludes solute species. The solid and gaseous phases, therefore, are composed of solvent only, and so transitions between these phases are not subject to colligative effects.

8.8.7: Osmosis and Osmotic Pressure of Solutions

A number of natural and synthetic materials exhibit *selective permeation*, meaning that only molecules or ions of a certain size, shape, polarity, charge, and so forth, are capable of passing through (permeating) the material. Biological cell membranes provide elegant examples of selective permeation in nature, while dialysis tubing used to remove metabolic wastes from blood is a more simplistic technological example. Regardless of how they may be fabricated, these materials are generally referred to as **semipermeable membranes**.

Consider the apparatus illustrated in Figure 8.8.7, in which samples of pure solvent and a solution are separated by a membrane that only solvent molecules may permeate. Solvent molecules will diffuse across the membrane in both directions. Since the concentration of *solvent* is greater in the pure solvent than the solution, these molecules will diffuse from the solvent side of the membrane to the solution side at a faster rate than they will in the reverse direction. The result is a net transfer of solvent molecules from the pure solvent to the solution. Diffusion-driven transfer of solvent molecules through a semipermeable membrane is a process known as **osmosis**.

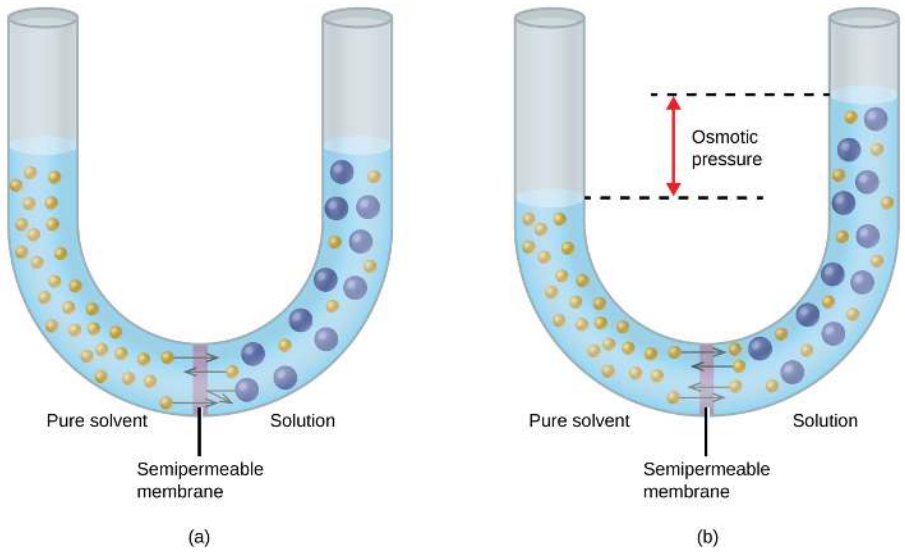


Figure 8.8.7: (a) A solution and pure solvent are initially separated by an osmotic membrane. (b) Net transfer of solvent molecules to the solution occurs until its osmotic pressure yields equal rates of transfer in both directions.

When osmosis is carried out in an apparatus like that shown in Figure 8.8.7, the volume of the solution increases as it becomes diluted by accumulation of solvent. This causes the level of the solution to rise, increasing its hydrostatic pressure (due to the weight of the column of solution in the tube) and resulting in a faster transfer of solvent molecules back to the pure solvent side. When the pressure reaches a value that yields a reverse solvent transfer rate equal to the osmosis rate, bulk transfer of solvent ceases. This pressure is called the **osmotic pressure** (Π) of the solution. The osmotic pressure of a dilute solution is related to its solute molarity, M, and absolute temperature, T, according to the equation

$$\Pi = MRT \tag{8.8.2}$$

where R is the universal gas constant.

Example 8.8.8: Calculation of Osmotic Pressure

Assuming ideal solution behavior, what is the osmotic pressure (atm) of a 0.30 M solution of glucose in water that is used for intravenous infusion at body temperature, 37 °C?

Solution

Find the osmotic pressure, Π, using Equation 8.8.2 (\(\ce{Π = MRT}\)), where T is on the Kelvin scale (310 K) and the value of R is expressed in appropriate units (0.08206 L atm/mol K).

$$\begin{aligned}\Pi &= MRT \\ &= 0.30 mol/L \times 0.08206 Latm/molK \times 310 K \\ &= 7.6 atm\end{aligned}$$

Exercise 8.8.8

Assuming ideal solution behavior, what is the osmotic pressure (atm) a solution with a volume of 0.750 L that contains 5.0 g of methanol, CH_3OH, in water at 37 °C?

Answer

5.3 atm

If a solution is placed in an apparatus like the one shown in Figure 8.8.8, applying pressure greater than the osmotic pressure of the solution reverses the osmosis and pushes solvent molecules from the solution into the pure solvent. This technique of reverse osmosis is used for large-scale desalination of seawater and on smaller scales to produce high-purity tap water for drinking.

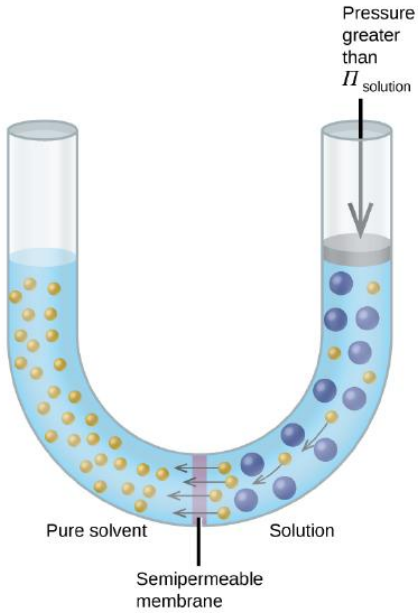


Figure 8.8.8: Applying a pressure greater than the osmotic pressure of a solution will reverse osmosis. Solvent molecules from the solution are pushed into the pure solvent.

Chemistry in Everyday Life: Reverse Osmosis Water Purification

In the process of osmosis, diffusion serves to move water through a semipermeable membrane from a less concentrated solution to a more concentrated solution. Osmotic pressure is the amount of pressure that must be applied to the more concentrated solution to cause osmosis to stop. If greater pressure is applied, the water will go from the more concentrated solution to a less concentrated (more pure) solution. This is called reverse osmosis. Reverse osmosis (RO) is used to purify water in many applications, from desalination plants in coastal cities, to water-purifying machines in grocery stores (Figure

8.8.9), and smaller reverse-osmosis household units. With a hand-operated pump, small RO units can be used in third-world countries, disaster areas, and in lifeboats. Our military forces have a variety of generator-operated RO units that can be transported in vehicles to remote locations.



(a) (b)

Figure 8.8.9: Reverse osmosis systems for purifying drinking water are shown here on (a) small and (b) large scales. (credit a: modification of work by Jerry Kirkhart; credit b: modification of work by Willard J. Lathrop)

Examples of osmosis are evident in many biological systems because cells are surrounded by semipermeable membranes. Carrots and celery that have become limp because they have lost water can be made crisp again by placing them in water. Water moves into the carrot or celery cells by osmosis. A cucumber placed in a concentrated salt solution loses water by osmosis and absorbs some salt to become a pickle. Osmosis can also affect animal cells. Solute concentrations are particularly important when solutions are injected into the body. Solutes in body cell fluids and blood serum give these solutions an osmotic pressure of approximately 7.7 atm. Solutions injected into the body must have the same osmotic pressure as blood serum; that is, they should be **isotonic** with blood serum. If a less concentrated solution, a **hypotonic** solution, is injected in sufficient quantity to dilute the blood serum, water from the diluted serum passes into the blood cells by osmosis, causing the cells to expand and rupture. This process is called **hemolysis**. When a more concentrated solution, a hypertonic solution, is injected, the cells lose water to the more concentrated solution, shrivel, and possibly die in a process called **crenation**. These effects are illustrated in Figure 8.8.9.

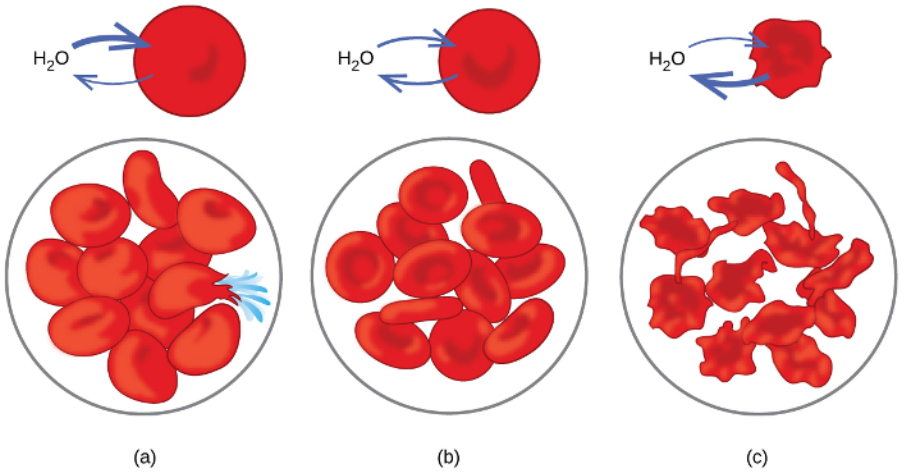


Figure 8.8.9 Red blood cell membranes are water permeable and will (a) swell and possibly rupture in a hypotonic solution; (b) maintain normal volume and shape in an isotonic solution; and (c) shrivel and possibly die in a hypertonic solution. (credit a/b/c: modifications of work by “LadyofHats”/Wikimedia commons)

8.8.8: Determination of Molar Masses

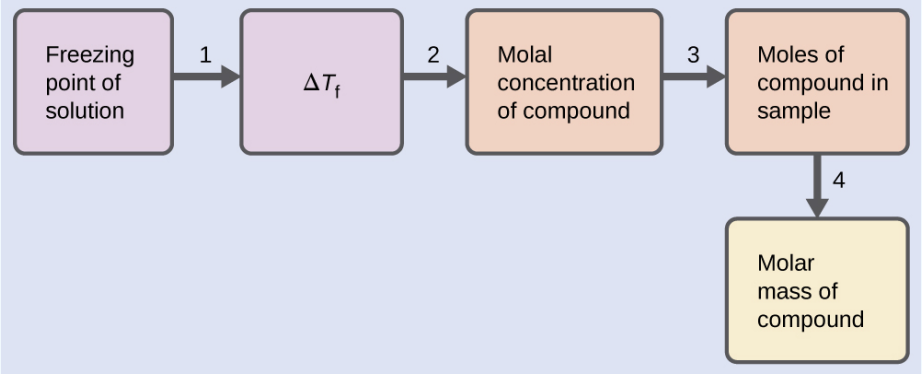
Osmotic pressure and changes in freezing point, boiling point, and vapor pressure are directly proportional to the number of solute species present in a given amount of solution. Consequently, measuring one of these properties for a solution prepared using a known mass of solute permits determination of the solute’s molar mass.

Example 8.8.9: Determination of a Molar Mass from a Freezing Point Depression

A solution of 4.00 g of a nonelectrolyte dissolved in 55.0 g of benzene is found to freeze at 2.32 °C. Assuming ideal solution behavior, what is the molar mass of this compound?

Solution

Solve this problem using the following steps.



Step 1. Determine the change in freezing point from the observed freezing point and the freezing point of pure benzene (Table 8.8.1.

$$\Delta T_f = 5.5°C - 2.32°C = 3.2°C$$

Step 2. Determine the molal concentration from Kf, the freezing point depression constant for benzene (Table 8.8.1), and ΔT_f.

$$\Delta T_f = K_f m$$

$$m = \frac{\Delta T_f}{K_f} = \frac{3.2°C}{5.12°Cm^{-1}} = 0.63m$$

Step 3. Determine the number of moles of compound in the solution from the molal concentration and the mass of solvent used to make the solution.

$$\text{Moles of solute} = \frac{0.63 \text{ mol solute}}{1.00 \cancel{\text{ kg solvent}}} \times 0.0550 \cancel{\text{ kg solvent}} = 0.035mol$$

Step 4. Determine the molar mass from the mass of the solute and the number of moles in that mass.

$$\text{Molar mass} = \frac{4.00 \text{ g}}{0.035 \text{ mol}} = 1.1 \times 10^2 \text{ g / mol}$$

Exercise 8.8.9

A solution of 35.7 g of a nonelectrolyte in 220.0 g of chloroform has a boiling point of 64.5 °C. Assuming ideal solution behavior, what is the molar mass of this compound?

Answer

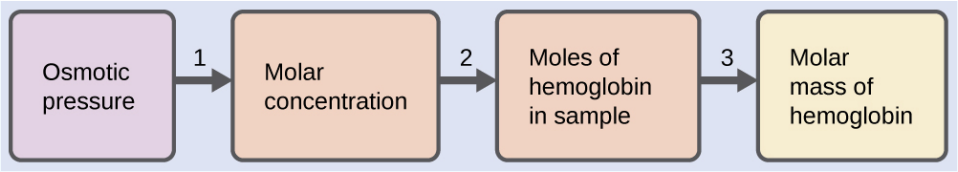
1.8 \times 10^{2} g/mol

Example 8.8.10: Determination of a Molar Mass from Osmotic Pressure

A 0.500 L sample of an aqueous solution containing 10.0 g of hemoglobin has an osmotic pressure of 5.9 torr at 22 °C. Assuming ideal solution behavior, what is the molar mass of hemoglobin?

Solution

Here is one set of steps that can be used to solve the problem:



Step 1. Convert the osmotic pressure to atmospheres, then determine the molar concentration from the osmotic pressure.

$$\Pi = \frac{5.9 \text{ torr } \times 1 atm}{760 \text{ torr}} = 7.8 \times 10^{-3} atm$$

$$\Pi = MRT$$

$$M = \frac{\Pi}{RT} = \frac{7.8 \times 10^{-3} atm}{(0.08206 L atm/mol K)(295 K)} = 3.2 \times 10^{-4} M$$

Step 2. Determine the number of moles of hemoglobin in the solution from the concentration and the volume of the solution.

$$\text{moles of hemoglobin } = \frac{3.2 \times 10^{-4} mol}{1 \text{ L solution}} \times 0.500 \text{ L solution} = 1.6 \times 10^{-4} \text{ mol}$$

Step 3. Determine the molar mass from the mass of hemoglobin and the number of moles in that mass.

$$\text{molar mass } = \frac{10.0 \text{ g}}{1.6 \times 10^{-4} \text{ mol}} = 6.2 \times 10^{4} \text{ g / mol}$$

? Exercise 8.8.10

Assuming ideal solution behavior, what is the molar mass of a protein if a solution of 0.02 g of the protein in 25.0 mL of solution has an osmotic pressure of 0.56 torr at 25 °C?

Answer

3 \times 10^{4} g/mol

8.8.9: Colligative Properties of Electrolytes

As noted previously in this module, the colligative properties of a solution depend only on the number, not on the identity, of solute species dissolved. The concentration terms in the equations for various colligative properties (freezing point depression, boiling point elevation, osmotic pressure) pertain to *all solute species present in the solution*. For the solutions considered thus far in this chapter, the solutes have been nonelectrolytes that dissolve physically without dissociation or any other accompanying process. Each molecule that dissolves yields one dissolved solute molecule. The dissolution of an electroyte, however, is not this simple, as illustrated by the two common examples below:

$$\text{dissociation} \quad NaCl(s) \longrightarrow Na^+(aq) + Cl^-(aq)$$

$$\text{ionization} \quad HCl(aq) + H_2O(l) \longrightarrow Cl^-(aq) + H3O^+(aq)$$

Considering the first of these examples, and assuming complete dissociation, a 1.0 *m* aqueous solution of NaCl contains 2.0 mole of ions (1.0 mol Na^+ and 1.0 mol Cl^-) per each kilogram of water, and its freezing point depression is expected to be

$$\Delta T_f = 2.0 mol \text{ ions } / kg \text{ water } \times 1.86 ^\circ C kg \text{ water } / mol \text{ ion } = 3.7 ^\circ C.$$

When this solution is actually prepared and its freezing point depression measured, however, a value of 3.4 °C is obtained. Similar discrepancies are observed for other ionic compounds, and the differences between the measured and expected colligative property

values typically become more significant as solute concentrations increase. These observations suggest that the ions of sodium chloride (and other strong electrolytes) are not completely dissociated in solution.

To account for this and avoid the errors accompanying the assumption of total dissociation, an experimentally measured parameter named in honor of Nobel Prize-winning German chemist Jacobus Henricus van 't Hoff is used. The van 't Hoff factor (i) is defined as the ratio of solute particles in solution to the number of formula units dissolved:

$$i = \frac{\text{moles of particles in solution}}{\text{moles of formula units dissolved}}$$

Values for measured van 't Hoff factors for several solutes, along with predicted values assuming complete dissociation, are shown in Table 8.8.2.

Table 8.8.2: Predicated and Measured van't Hoff Factors for Several 0.050 *m* Aqueous Solutions

Formula unit	Classification	Dissolution products	*i* (predicted)	*i* (measured)
$C_{12}H_{22}O_{11}$ (glucose)	Nonelectrolyte	$C_{12}H_{22}O_{11}$	1	1.0
NaCl	Strong electrolyte	Na^+, Cl^-	2	1.9
HCl	Strong electrolyte (acid)	H_3O^+, Cl^-	2	1.9
$MgSO_4$	Strong electrolyte	Mg^{2+}, SO_4^{2-},	2	1.3
$MgCl_2$	Strong electrolyte	Mg^{2+}, $2Cl^-$	3	2.7
$FeCl_3$	Strong electrolyte	Fe^{3+}, $3Cl^-$	4	3.4

In 1923, the chemists Peter Debye and Erich Hückel proposed a theory to explain the apparent incomplete ionization of strong electrolytes. They suggested that although interionic attraction in an aqueous solution is very greatly reduced by solvation of the ions and the insulating action of the polar solvent, it is not completely nullified. The residual attractions prevent the ions from behaving as totally independent particles (Figure 8.8.11). In some cases, a positive and negative ion may actually touch, giving a solvated unit called an ion pair. Thus, the activity, or the effective concentration, of any particular kind of ion is less than that indicated by the actual concentration. Ions become more and more widely separated the more dilute the solution, and the residual interionic attractions become less and less. Thus, in extremely dilute solutions, the effective concentrations of the ions (their activities) are essentially equal to the actual concentrations. Note that the van't Hoff factors for the electrolytes in Table 8.8.2 are for 0.05 *m* solutions, at which concentration the value of *i* for NaCl is 1.9, as opposed to an ideal value of 2.

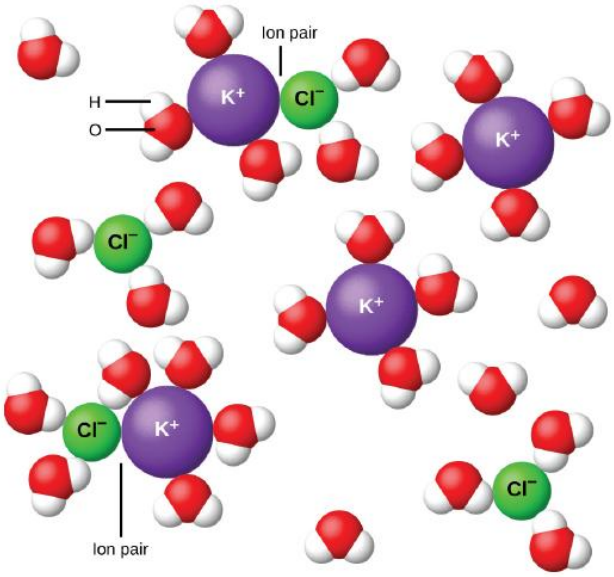


Figure 8.8.11: Dissociation of ionic compounds in water is not always complete due to the formation of ion pairs.

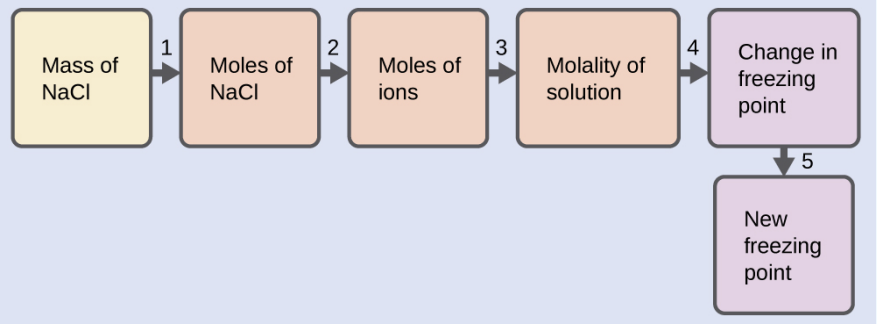
https://chem.libretexts.org/@go/page/449309

Example 8.8.11: The Freezing Point of a Solution of an Electrolyte

The concentration of ions in seawater is approximately the same as that in a solution containing 4.2 g of NaCl dissolved in 125 g of water. Use this information and a predicted value for the van't Hoff factor (Table **8.8.2**) to determine the freezing temperature the solution (assume ideal solution behavior).

Solution

Solve this problem using the following series of steps.



1. Step 1. *Convert from grams to moles of NaCl using the molar mass of NaCl in the unit conversion factor.*
   Result: 0.072 mol NaCl
2. Step 2. *Determine the number of moles of ions present in the solution using the number of moles of ions in 1 mole of NaCl as the conversion factor (2 mol ions/1 mol NaCl).*
   Result: 0.14 mol ions
3. Step 3. *Determine the molality of the ions in the solution from the number of moles of ions and the mass of solvent, in kilograms.*
   Result: 1.2 *m*
4. Step 4. *Use the direct proportionality between the change in freezing point and molal concentration to determine how much the freezing point changes.*
   Result: 2.1 °C
5. Step 5. *Determine the new freezing point from the freezing point of the pure solvent and the change.*
   Result: −2.1 °C

Check each result as a self-assessment, taking care to avoid rounding errors by retaining guard digits in each step's result for computing the next step's result.

Exercise 8.8.11

Assuming complete dissociation and ideal solution behavior, calculate the freezing point of a solution of 0.724 g of $CaCl_2$ in 175 g of water.

Answer

−0.208 °C

This page titled 8.8: Osmosis, Diffusion and Dialysis is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **11.4: Colligative Properties** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

8.9: Health Connections- Oxygen in the Body

The air we breathe is made up of various gases, 21% of which is oxygen. Therefore, a patient who is receiving no supplemental oxygen therapy is still receiving oxygen from the air. This amount of oxygen is adequate provided that the patient's airway is not compromised and there is sufficient hemoglobin in the blood. The cardiovascular system must also be intact and able to circulate blood to all body tissues. If any of these systems fail, the patient will require supplemental oxygen to increase the likelihood that adequate levels of oxygen will reach all vital body tissues necessary to sustain life.

Oxygen in the Blood

Hemoglobin (Hgb) holds oxygen in reserve until the metabolic demands of the body require more oxygen. The Hgb then moves the oxygen to the plasma for transport to the tissues. The body's demand for oxygen is affected by activity, metabolic status, temperature, and level of anxiety. The ability of Hgb to move the oxygen to the tissues depends on a number of factors, such as oxygen supply, ventilatory effectiveness, nutrition, cardiac output, hemoglobin level, smoking, drug use, and underlying disease. Any one of these factors can potentially impede the supply and transport of oxygen to the tissues.

Measurement of Oxygen in the Blood

The vast majority of oxygen carried in the blood is attached to hemoglobin and can be assessed by monitoring the oxygen saturation through pulse oximetry (SpO_2).The target range for oxygen saturation as measured by blood analysis (SaO_2), such as arterial blood gas, is 92% to 98% for a normal adult. **Arterial blood gas (ABG)** is the analysis of an arterial blood sample to evaluate the adequacy of ventilation, oxygen delivery to the tissues, and acid-base balance status (Simpson, 2004). For patients with COPD, the target SaO_2 range is 88% to 92% (Alberta Health Services, 2015; British Thoracic Society, 2008; Kane et al., 2013). Only about 3% of the oxygen carried in the blood is dissolved in the plasma, which can be assessed by looking at the partial pressure of oxygen in the blood through blood gas analysis (PaO_2). The normal PaO_2 of a healthy adult is 80 to 100 mmHg. The SpO_2 is more clinically significant than the PaO_2in determining the oxygen content of the blood.

Oxygen is considered a medication and therefore requires continuous monitoring of the dose, concentration, and side effects to ensure its safe and effective use (Alberta Health Services, 2015). Oxygen therapy may be indicated for hypoxemia and hypoxia.

Understanding Hypoxemia and Hypoxia

Although the terms *hypoxemia* and *hypoxia* are often used interchangeably, they do not mean the same thing. **Hypoxemia** is a condition where arterial oxygen tension or partial pressure of oxygen (PaO_2) is below normal (<80 mmHg). Hypoxemia is the inadequate supply of oxygen in the arterial blood. **Hypoxia** is the reduction of oxygen supply at the tissue level, which is not measured directly by a laboratory value (Metrovic, 2014), but by pulse oximetry and SpO_2 (British Thoracic Society, 2008).

Generally, the presence of hypoxemia suggests that hypoxia exists. However, hypoxia may not be present in a patient with hypoxemia if the patient is able to compensate for a low PaO_2 by increasing oxygen supply. This is usually achieved by increasing cardiac output (by raising the heart rate) or by decreasing tissue oxygen consumption. Conversely, patients who do not show signs of hypoxemia may be hypoxic if oxygen delivery to the tissues is diminished or if the tissues are unable to adequately use the oxygen.

Hypoxemia is the most common cause of tissue hypoxia, and if the correct diagnosis is made, it is readily treatable.

The Vancouver Coastal Health Authority (2015) lists three causes of hypoxemia: deadspace and shunts, low inspired oxygen tension, and alveolar hypoventilation.

Deadspace and Shunts

Ventilation and perfusion are not always equal between the alveoli and pulmonary capillaries. There is sometimes too much perfusion and not enough ventilation in some areas of the lungs, causing a shunt where the blood is unable to pick up oxygen and unload carbon dioxide. In other areas of the lungs, there may be too much ventilation and not enough perfusion, causing deadspace where oxygen is unable to diffuse into the blood.

Low Inspired Oxygen Tension

Hypoxemia can be caused by breathing air at pressures less than atmospheric pressure, such as at high altitudes or in an enclosed space with inadequate ventilation. The enclosed space may be especially hazardous if there is a low concentration of oxygen or if it contains toxic gases.

Alveolar Hypoventilation

If a patient hypoventilates, the level of oxygen in the alveoli will fall, and the level of carbon dioxide will increase. Hypoxemia occurs because less oxygen is moved into the pulmonary blood flow.

Examples of medical conditions that cause hypoxemia include:

- Asthma
- COPD
- Heart failure
- Pleural effusions
- Pneumonia
- Pneumothorax
- Pulmonary edema
- Pulmonary emboli

With hypoxia, there is inadequate transport of oxygen to the cells or tissues, either because of obstruction, secretions, or tumours in the lungs; hypoventilation due to disease, injury to the respiratory system, or medications; or poor blood flow due to a compromised circulatory system (British Thoracic Society, 2008). Hypoxia related to anemia or circulatory system compromise, such as decreased cardiac output, will respond poorly to oxygen therapy, and other appropriate interventions should be considered.

Hypoxia is a medical emergency (Alberta Health Services, 2015). Oxygen therapy will:

- Decrease the work of breathing in patients with respiratory or cardiovascular conditions, which may prevent respiratory and muscle fatigue (Jardins & Burton, 2011).
- Decrease cardiopulmonary workload by reducing high cardiopulmonary demand (Perry et al., 2014). For example, patients with left ventricular failure benefit from additional oxygen to the tissues because the heart cannot provide enough oxygen to the tissues due to decreased cardiac output.
- Support post-operative recovery, and may be ordered for a specific time frame at a specific rate while the patient recovers from the surgical procedure.

Critical Thinking Exercises

1. How do you know if your patient is hypoxic or hypoxemic? Please explain.
2. Why would the post-surgical patient require supplemental oxygen?

This page titled 8.9: Health Connections- Oxygen in the Body is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Glynda Rees Doyle and Jodie Anita McCutcheon (BCcampus) via source content that was edited to the style and standards of the LibreTexts platform.

- **5.2: Principles** by Glynda Rees Doyle and Jodie Anita McCutcheon is licensed CC BY 4.0. Original source: https://opentextbc.ca/clinicalskills/.

8.10: Case Study- The Vital Breath – Kinetic Molecular Theory in Respiratory Care

Introduction: In the nuanced practice of respiratory therapy, the principles of Kinetic Molecular Theory (KMT) are both theoretical cornerstones and practical tools for understanding and explaining patient treatments. This case study focuses on how respiratory therapists employ KMT to elucidate the gas exchange process in the lungs during oxygen therapy.

Scenario: At Breathe Easy Respiratory Clinic, Mark, an experienced respiratory therapist, is preparing to administer oxygen therapy to a young patient, Emma, who is struggling with pneumonia. To ease Emma's anxiety about the mask and the machine, Mark gently explains how the invisible gases will help her breathe more easily. He brings in the Kinetic Molecular Theory to paint a picture of the tiny oxygen molecules traveling into her lungs and finding their way into her bloodstream.

Kinetic Molecular Theory and Gas Behavior: Mark describes how, according to KMT, the oxygen molecules she breathes in are like tiny, fast-moving particles that spread out and zip through the air sacs of her lungs to where they're needed most. He explains that these molecules move from the high concentration in her oxygen mask to mingle with the lower concentration in her blood, highlighting the tireless and random motion that makes life-sustaining gas exchange possible.

Case Study Questions:

1. **How does the Kinetic Molecular Theory explain the behavior of gases?**
2. **Why is understanding intermolecular forces important in intravenous fluid selection?**

Hands-On Classroom Activities:

1. **Gas Behavior Simulation:** In the "Gas Behavior Simulation," students will use balloons to simulate the behavior of gases, measuring changes in pressure to gain a practical understanding of gas exchange in the lungs. This hands-on activity aims to illustrate the principles of gas laws and how they apply to respiratory physiology.
2. **Fluid Properties Lab:** The "Fluid Properties Lab" invites students to observe and compare the viscosity and osmotic behavior of various liquids. By conducting this comparison, students aim to establish a connection between the physical properties of fluids and the critical process of fluid selection in healthcare settings.

Conclusion: For Emma and many others at the Breathe Easy Respiratory Clinic, Mark's ability to translate the Kinetic Molecular Theory into understandable and relatable explanations demystifies the oxygen therapy process. His personal approach both comforts and educates patients on the science behind their treatment. This case study illustrates how fundamental concepts like KMT and intermolecular forces, when understood and communicated effectively, become integral to providing compassionate and informed patient care in the medical field.

8.10: Case Study- The Vital Breath – Kinetic Molecular Theory in Respiratory Care is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

8.E: Exercises

Multiple-Choice Questions

1. Which of the following is *not* a postulate of the kinetic molecular theory of gases?
    a. The average kinetic energy of the gas molecules is proportional to the absolute temperature.
    b. Gas particles attract and repel one another.
    c. The size of the gas particles is negligible compared to the distances between them.
    d. Pressure arises due to the collisions between gas particles and the walls of the container.
2. What is the SI unit for pressure?
    a. Atmosphere
    b. Pounds per square inch
    c. Bar
    d. Pascal
3. Boyle's law relates which two variables?
    a. Volume and pressure
    b. Volume and temperature
    c. Pressure and temperature
    d. Moles and temperature
4. If a 2.0 L sample of a gas at 25 °C has a pressure of 2.4 atm, what is the pressure of this gas if its volume is decreased to 0.50 L at 25 °C?
    a. 0.60 atm
    b. 2.4 atm
    c. 7.2 atm
    d. 9.6 atm
5. Which of the following is the weakest intermolecular force?
    a. Dipole-dipole attractions
    b. Ion-dipole interactions
    c. Dispersion forces
    d. Hydrogen bonding
6. You dissolve a solid in a glass of water and feel the glass heat up. What do you know about the dissolution process?
    a. The process is exothermic.
    b. The process is endothermic.
    c. The water molecules slow down on average.
    d. Weaker bonds were formed compared to the bonds that were broken.
7. Which of the following compounds is a strong electrolyte?
    a. Sucrose
    b. Ethanol

c. Hydrochloric acid

d. Ammonia

8. Molarity is defined as moles of solute divided by what?

    a. Mass of solution

    b. Mass of solvent

    c. Liters of solvent

    d. Liters of solution

9. A 0.200 L solution contains 0.0200 moles of sodium chloride. What is the molarity of sodium chloride in this solution?

    a. 0.00400 M

    b. 0.100 M

    c. 0.220 M

    d. 10.0 M

10. If a hypotonic solution is injected into the bloodstream, which of the following will occur?

    a. Red blood cells will shrivel

    b. Hemolysis

    c. Both a and b

    d. Neither a nor b

Warm-up problems

1. Car tires typically have a pressure range of 32–35 psi. If a tire has a pressure of 34 psi on a day when the temperature is 18.3 °C, what is the tire pressure (assuming no change in volume) if the temperature drops to 1.67 °C? Be sure to use the appropriate unit for temperature when solving this problem.
2. If a balloon has an initial pressure of 1.07 atm and a volume of 14.0 L, what is its pressure if the volume is decreased to 12.0 L, assuming a constant temperature and amount of gas?
3. Identify the intermolecular forces present in the following solids:

    a. CH_3CH_2OH

    b. $CH_3CH_2CH_3$

    c. CH_3CH_2Cl

4. Identify the intermolecular forces present in the following solids:

    a. HCl

    b. H_2O

    c. CO_2

5. Arrange each of the following sets of compounds in order of increasing boiling point:

    a. HCl, H_2O, SiH_4

    b. F_2, Cl_2, Br_2

6. Arrange each of the following sets of compounds in order of increasing boiling point:

    a. CH_4, C_2H_6, C_3H_8

    b. O_2, NO, N_2

7. What is the expected electrical conductivity of the following solutions?

    a. NaOH(aq)

    b. HCl(aq)

8. What is the expected electrical conductivity of the following solutions?

a. $C_6H_{12}O_6$(aq) (glucose)
b. NH_3(aq)

9. Indicate the most important type of intermolecular attraction responsible for solvation in each of the following solutions:
   a. Methanol (CH_3OH) dissolved in ethanol (C_2H_5OH)
   b. Methane (CH_4) dissolved in benzene (C_6H_6)
10. Indicate the most important type of intermolecular attraction responsible for solvation in each of the following solutions:
   a. The polar halocarbon CF_2Cl_2 dissolved in the polar halocarbon $CF_2ClCFCl_2$
   b. O_2(l) in N_2(l)
11. Determine the molarity for each of the following solutions:
   a. 10.5 kg of $Na_2SO_4{\cdot}_{10}H_2O$ in 18.60 L of solution
   b. 7.0 × 10−3 mol of I_2 in 100.0 mL of solution
   c. 1.8 × 104 mg of HCl in 0.075 L of solution
12. Determine the molarity for each of the following solutions:
   a. 1.457 mol KCl in 1.500 L of solution
   b. 0.515 g of H_2SO_4 in 1.00 L of solution
   c. 20.54 g of aluminum nitrate in 1575 mL of solution
13. Determine the molarity for each of the following solutions:
   a. 2.76 kg of $CuSO_4{\cdot}5H_2O$ in 1.45 L of solution
   b. 0.005653 mol of Br_2 in 10.00 mL of solution
   c. 0.000889 g of glycine ($C_2H_5NO_2$) in 1.05 mL of solution
14. What is the mass of solute in 0.500 L of 0.30 M glucose ($C_6H_{12}O_6$) used for intravenous injection?
15. What is the mass of solute in 200.0 mL of a 1.556 M solution of KBr?
16. An experiment in a general chemistry laboratory calls for a 2.00 M solution of HCl. How many mL of 11.9 M HCl would be required to make 250. mL of 2.00 M HCl?
17. What is the final concentration of the solution produced when 225.5 mL of a 0.09988 M solution of Na_2CO_3 is allowed to evaporate until the solution volume is reduced to 45.00 mL?
18. Define a hypotonic solution.
19. Define a hypertonic solution.

Medium

1. If a balloon with a volume of 13.8 L at a temperature of 23.0 °C and a pressure of 1.0 atm is allowed to rise to a location in the atmosphere where the pressure is 0.75 atm and the temperature is 18.5 °C, what is the balloon's new volume?
2. A gas sample has an initial volume of 20.0 mL at 25.0 °C and 0.985 atm. If the pressure is increased to 1.98 atm and the volume is decreased to 10.2 mL, what is the gas sample's final temperature (in kelvin units)? Assume the amount of gas remains constant.
3. What mass of NaCl is required to make 500.0 mL of a 0.250 M solution of NaCl?
4. Calculate the volume of a 0.530 M solution of HCl needed to make 250.0 mL of a 0.125 M solution of HCl.
5. Why do the boiling points of the noble gases increase in the order He < Ne < Ar < Kr < Xe?
6. Neon and HF have approximately the same molecular masses. Explain why the boiling points of neon and HF differ.
7. The melting point of H_2O is 0 °C. Would you expect the melting point of H_2S to be −85 °C, 0 °C, or 185 °C? Explain your answer.
8. When KNO_3 is dissolved in water, the resulting solution is significantly colder than the water was originally.
   a. Is the dissolution of KNO_3 an endothermic or exothermic process?
   b. What conclusions can you draw about the intermolecular attractions involved in the process?
9. What does it mean when we say that a 200 mL sample and a 400 mL sample of a salt solution have the same molarity? In what ways are the two samples identical? In what ways are the two samples different?
10. Explain reverse osmosis and how this can be used to purify water.

11. If red blood cells added to a solution are observed to shrivel up, does the solution have a higher or lower salt concentration than the red blood cells? Explain your answer.

Challenge

1. An oxygen tank for a patient has a volume of 10.0 L and contains oxygen at a pressure of 2015 psi. Assuming no change in the oxygen temperature, determine how long (in minutes) this tank of oxygen will last if the oxygen is delivered at a pressure of 14.7 psi (atmospheric pressure) and a flow rate of 12.0 L/min. (Hint: first calculate the volume of oxygen at 14.7 psi).
2. A common intravenous solution is 0.9% saline, which contains 0.900 g of NaCl in 100.0 mL of solution. This solution is commonly used as it is isotonic with blood. Patients suffering from hyponatremia (where the sodium concentration in the blood is less than normal) are sometimes treated with 3% saline (3.00 g NaCl in 100.0 mL of solution). Serum levels are typically reported in units of mEq/L or milliequivalents per liter. As NaCl produces one sodium ion per formula unit of NaCl, mEq/L for sodium is equivalent to mmol/L. Determine the molarity and mEq/L sodium ion concentrations for 0.9% and 3% saline.

Health-Related Questions

1. Calculate the molarity for each of the following solutions:
    a. 0.195 g of cholesterol ($C_{27}H_{46}O$) in 0.100 L of serum, the average concentration of cholesterol in human serum
    b. 4.25 g of NH_3 in 0.500 L of solution, the concentration of NH_3 in household ammonia
    c. 1.49 kg of isopropyl alcohol (C_3H_7OH) in 2.50 L of solution, the concentration of isopropyl alcohol in rubbing alcohol
    d. 0.029 g of I_2 in 0.100 L of solution, the solubility of I_2 in water at 20 °C
2. Calculate the molarity for each of the following solutions:
    a. 293 g HCl in 666 mL of solution, a concentrated HCl solution
    b. 2.026 g $FeCl_3$ in 0.1250 L of a solution used as an unknown in general chemistry laboratories
    c. 0.001 mg Cd^{2+} in 0.100 L, the maximum permissible concentration of cadmium in drinking water
    d. 0.0079 g $C_7H_5SNO_3$ in one ounce (29.6 mL), the concentration of saccharin in a diet soft drink

8.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

9: Acids and Bases

9.1: What are Acids and Bases?

9.2: pH and pOH

9.3: Acid-Base Balance

9.4: Case Study- Navigating the Delicate pH Spectrum in Intensive Care

9.E: Exercises

9: Acids and Bases is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

9.1: What are Acids and Bases?

Learning Objectives

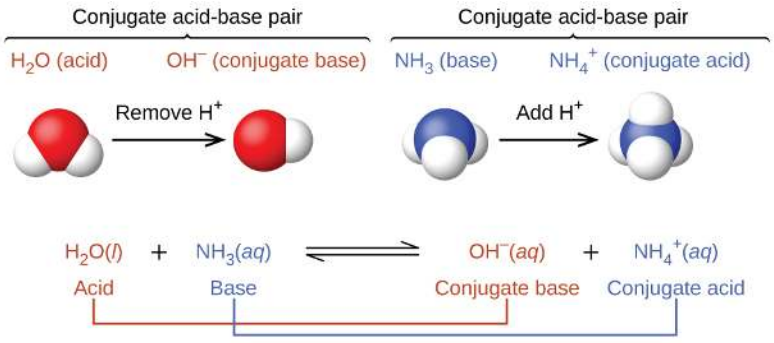
By the end of this section, you will be able to:

- Identify acids, bases, and conjugate acid-base pairs according to the Brønsted-Lowry definition
- Write equations for acid and base ionization reactions
- Use the ion-product constant for water to calculate hydronium and hydroxide ion concentrations
- Describe the acid-base behavior of amphiprotic substances

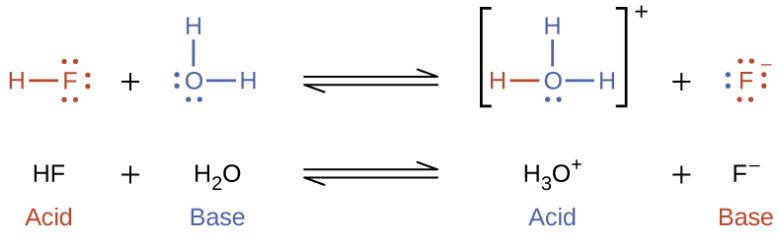
The acid-base reaction class has been studied for quite some time. In 1680, Robert Boyle reported traits of acid solutions that included their ability to dissolve many substances, to change the colors of certain natural dyes, and to lose these traits after coming in contact with alkali (base) solutions. In the eighteenth century, it was recognized that acids have a sour taste, react with limestone to liberate a gaseous substance (now known to be CO_2), and interact with alkalis to form neutral substances. In 1815, Humphry Davy contributed greatly to the development of the modern acid-base concept by demonstrating that hydrogen is the essential constituent of acids. Around that same time, Joseph Louis Gay-Lussac concluded that acids are substances that can neutralize bases and that these two classes of substances can be defined only in terms of each other. The significance of hydrogen was reemphasized in 1884 when Svante Arrhenius defined an acid as a compound that dissolves in water to yield hydrogen cations (now recognized to be hydronium ions) and a base as a compound that dissolves in water to yield hydroxide anions.

Johannes Brønsted and Thomas Lowry proposed a more general description in 1923 in which acids and bases were defined in terms of the transfer of hydrogen ions, H^+. (Note that these hydrogen ions are often referred to simply as *protons*, since that subatomic particle is the only component of cations derived from the most abundant hydrogen isotope, ^1H.) A compound that donates a proton to another compound is called a Brønsted-Lowry acid, and a compound that accepts a proton is called a Brønsted-Lowry base. An acid-base reaction is, thus, the transfer of a proton from a donor (acid) to an acceptor (base).

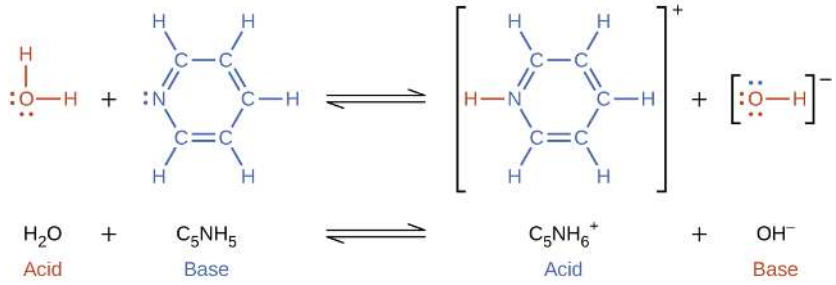
The concept of *conjugate pairs* is useful in describing Brønsted-Lowry acid-base reactions (and other reversible reactions, as well). When an acid donates H^+, the species that remains is called the **conjugate base** of the acid because it reacts as a proton acceptor in the reverse reaction. Likewise, when a base accepts H^+, it is converted to its **conjugate acid**. The reaction between water and ammonia illustrates this idea. In the forward direction, water acts as an acid by donating a proton to ammonia and subsequently becoming a hydroxide ion, OH^-, the conjugate base of water. The ammonia acts as a base in accepting this proton, becoming an ammonium ion, NH_4^+, the conjugate acid of ammonia. In the reverse direction, a hydroxide ion acts as a base in accepting a proton from ammonium ion, which acts as an acid.



The reaction between a Brønsted-Lowry acid and water is called acid ionization. For example, when hydrogen fluoride dissolves in water and ionizes, protons are transferred from hydrogen fluoride molecules to water molecules, yielding hydronium ions and fluoride ions:



Base ionization of a species occurs when it accepts protons from water molecules. In the example below, pyridine molecules, C_5NH_5, undergo base ionization when dissolved in water, yielding hydroxide and pyridinium ions:



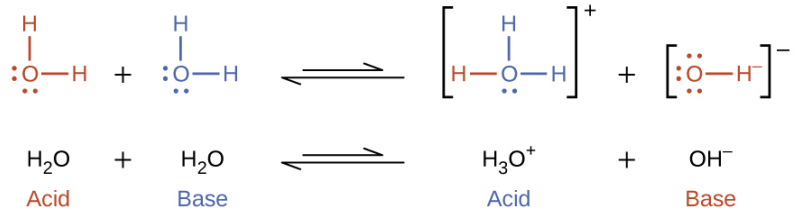
The preceding ionization reactions suggest that water may function as both a base (as in its reaction with hydrogen fluoride) and an acid (as in its reaction with ammonia). Species capable of either donating or accepting protons are called amphiprotic, or more generally, amphoteric, a term that may be used for acids and bases per definitions other than the Brønsted-Lowry one. The equations below show the two possible acid-base reactions for two amphiprotic species, bicarbonate ion and water:

$$HCO_3^-(aq) + H_2O(l) \rightleftharpoons CO_3^{2-}(aq) + H_3O^+(aq)$$

$$HCO_3^-(aq) + H_2O(l) \rightleftharpoons H_2CO_3(aq) + OH^-(aq)$$

The first equation represents the reaction of bicarbonate as an acid with water as a base, whereas the second represents reaction of bicarbonate as a base with water as an acid. When bicarbonate is added to water, both these equilibria are established simultaneously and the composition of the resulting solution may be determined through appropriate equilibrium calculations, as described later in this chapter.

In the liquid state, molecules of an amphiprotic substance can react with one another as illustrated for water in the equations below:



The process in which like molecules react to yield ions is called autoionization. Liquid water undergoes autoionization to a very slight extent; at 25 °C, approximately two out of every billion water molecules are ionized. The extent of the water autoionization process is reflected in the value of its equilibrium constant, the ion-product constant for water, K_w:

$$2\,H_2O(l) \rightleftharpoons H_3O^+(aq) + OH^-(aq) \tag{9.1.1}$$

with

$$K_w = [H_3O^+][OH^-] \tag{9.1.2}$$

The slight ionization of pure water is reflected in the small value of the equilibrium constant; at 25 °C, K_w has a value of 1.0×10^{-14}. The process is endothermic, and so the extent of ionization and the resulting concentrations of hydronium ion and

hydroxide ion increase with temperature. For example, at 100 °C, the value for K_w is about 5.6×10^{-13}, roughly 50 times larger than the value at 25 °C.

Example 9.1.1: Ion Concentrations in Pure Water

What are the hydronium ion concentration and the hydroxide ion concentration in pure water at 25 °C?

Solution

The autoionization of water yields the same number of hydronium and hydroxide ions. Therefore, in pure water, $[H_3O^+] = [OH^-] = x$. At 25 °C:

$$K_w = [H_3O^+]\,[OH^-] = (x)(x) = x^2 = 1.0 \times 10^{-14}$$

So:

$$x = [H_3O^+] = [OH^-] = \sqrt{1.0 \times 10^{-14}} = 1.0 \times 10^{-7} M$$

The hydronium ion concentration and the hydroxide ion concentration are the same, $1.0 \times 10^{-7}\,M$.

Exercise 9.1.1

The ion product of water at 80 °C is 2.4 \times 10^{−13}. What are the concentrations of hydronium and hydroxide ions in pure water at 80 °C?

Answer

$$[H_3O^+] = [OH^-] = 4.9 \times 10^{-7}\,M$$

Example 9.1.2: The Inverse Relation between $[H_3O^+]$ and $[OH^-]$

A solution of an acid in water has a hydronium ion concentration of $2.0 \times 10^{-6} M$. What is the concentration of hydroxide ion at 25 °C?

Solution

Use the value of the ion-product constant for water at 25 °C (Equations 9.1.1 and 9.1.2) to calculate the missing equilibrium concentration.

$$2\,H_2O\,(l) \rightleftharpoons H_3O^+\,(aq) + OH^-\,(aq)$$

with $K_w = [H_3O^+][OH^-]$.

Rearrangement of the K_w expression shows that $[OH^-]$ is inversely proportional to $[H_3O^+]$:

$$K_w = [H_3O^+]\,[OH^-] = (2.0 \times 10^{-6})\,(5.0 \times 10^{-9}) = 1.0 \times 10^{-14}$$

Compared with pure water, a solution of acid exhibits a higher concentration of hydronium ions (due to ionization of the acid) and a proportionally lower concentration of hydroxide ions. This may be explained via Le Chatelier's principle as a left shift in the water autoionization equilibrium resulting from the stress of increased hydronium ion concentration.

Substituting the ion concentrations into the K_w expression confirms this calculation, resulting in the expected value:

$$K_w = [H_3O^+][OH^-] = (2.0 \times 10^{-6})(5.0 \times 10^{-9}) = 1.0 \times 10^{-14}$$

Exercise 9.1.2

What is the hydronium ion concentration in an aqueous solution with a hydroxide ion concentration of 0.001 *M* at 25 °C?

Answer

$$[H_3O^+] = 1 \times 10^{-11}\ M$$

Example 9.1.3: Representing the Acid-Base Behavior of an Amphoteric Substance

Write separate equations representing the reaction of HSO_3^-

a. as an acid with OH^-
b. as a base with HI

Solution

a. $HSO_3^-(aq) + OH^-(aq) \rightleftharpoons SO_3^{2-}(aq) + H_2O(l)$
b. $HSO_3^-(aq) + HI(aq) \rightleftharpoons H_2SO_3(aq) + I^-(aq)$

Exercise 9.1.3

Write separate equations representing the reaction of $H_2PO_4^-$

a. as a base with HBr
b. as an acid with OH^-

Answer

a. $H_2PO_4^-(aq) + HBr(aq) \rightleftharpoons H_3PO_4(aq) + Br^-(aq)$
b. $H_2PO_4^-(aq) + OH^-(aq) \rightleftharpoons HPO_4^{2-}(aq) + H_2O(l)$

This page titled 9.1: What are Acids and Bases? is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **14.1: Brønsted-Lowry Acids and Bases** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

9.2: pH and pOH

Learning Objectives

By the end of this section, you will be able to:

- Explain the characterization of aqueous solutions as acidic, basic, or neutral
- Express hydronium and hydroxide ion concentrations on the pH and pOH scales
- Perform calculations relating pH and pOH

As discussed earlier, hydronium and hydroxide ions are present both in pure water and in all aqueous solutions, and their concentrations are inversely proportional as determined by the ion product of water (K_w). The concentrations of these ions in a solution are often critical determinants of the solution's properties and the chemical behaviors of its other solutes, and specific vocabulary has been developed to describe these concentrations in relative terms. A solution is neutral if it contains equal concentrations of hydronium and hydroxide ions; acidic if it contains a greater concentration of hydronium ions than hydroxide ions; and basic if it contains a lesser concentration of hydronium ions than hydroxide ions.

A common means of expressing quantities that may span many orders of magnitude is to use a logarithmic scale. One such scale that is very popular for chemical concentrations and equilibrium constants is based on the p-function, defined as shown where "X" is the quantity of interest and "log" is the base-10 logarithm:

$$pX = -\log X$$

The pH of a solution is therefore defined as shown here, where $[H_3O^+]$ is the molar concentration of hydronium ion in the solution:

$$pH = -\log [H_3O^+]$$

Rearranging this equation to isolate the hydronium ion molarity yields the equivalent expression:

$$[H_3O^+] = 10^{-pH}$$

Likewise, the hydroxide ion molarity may be expressed as a p-function, or pOH:

$$pOH = -\log [OH^-]$$

or

$$[OH^-] = 10^{-pOH}$$

Finally, the relation between these two ion concentration expressed as p-functions is easily derived from the K_w expression:

$$\begin{aligned} K_w &= [\mathrm{H_3O^+}]\,[\mathrm{OH^-}] \\ -\log K_w &= -\log \left([\mathrm{H_3O^+}]\,[\mathrm{OH^-}]\right) \\ &= -\log [\mathrm{H_3O^+}] + -\log [\mathrm{OH^-}] \\ pK_w &= pH + pOH \end{aligned} \tag{9.2.1}$$

At 25 °C, the value of K_w is 1.0×10^{-14}, and so:

$$14.00 = pH + pOH$$

As was demonstrated previously, the hydronium ion molarity in pure water (or any neutral solution) is 1.0×10^{-7} M at 25 °C. The pH and pOH of a neutral solution at this temperature are therefore:

$$pH = -\log [H_3O^+] = -\log \left(1.0 \times 10^{-7}\right) = 7.00$$

$$pOH = -\log [OH^-] = -\log \left(1.0 \times 10^{-7}\right) = 7.00$$

And so, *at this temperature*, acidic solutions are those with hydronium ion molarities greater than 1.0×10^{-7} M and hydroxide ion molarities less than 1.0×10^{-7} M (corresponding to pH values less than 7.00 and pOH values greater than 7.00). Basic solutions are

those with hydronium ion molarities less than 1.0×10^{-7} M and hydroxide ion molarities greater than 1.0×10^{-7} M (corresponding to pH values greater than 7.00 and pOH values less than 7.00).

Since the autoionization constant K_w is temperature dependent, these correlations between pH values and the acidic/neutral/basic adjectives will be different at temperatures other than 25 °C. For example, Exercise **9.2.1** showed the hydronium molarity of pure water at 80 °C is 4.9×10^{-7} M, which corresponds to pH and pOH values of:

$$pH = -\log\left[H_3O^+\right] = -\log\left(4.9 \times 10^{-7}\right) = 6.31$$

$$pOH = -\log\left[OH^-\right] = -\log\left(4.9 \times 10^{-7}\right) = 6.31$$

At this temperature, then, neutral solutions exhibit pH = pOH = 6.31, acidic solutions exhibit pH less than 6.31 and pOH greater than 6.31, whereas basic solutions exhibit pH greater than 6.31 and pOH less than 6.31. This distinction can be important when studying certain processes that occur at other temperatures, such as enzyme reactions in warm-blooded organisms at a temperature around 36–40 °C. Unless otherwise noted, references to pH values are presumed to be those at 25 °C (Table **9.2.1**).

Table **9.2.1**: Summary of Relations for Acidic, Basic and Neutral Solutions

Classification	Relative Ion Concentrations	pH at 25 °C
acidic	$[H_3O^+] > [OH^-]$	pH < 7
neutral	$[H_3O^+] = [OH^-]$	pH = 7
basic	$[H_3O^+] < [OH^-]$	pH > 7

Figure **9.2.1**: shows the relationships between $[H_3O^+]$, $[OH^-]$, pH, and pOH for solutions classified as acidic, basic, and neutral.

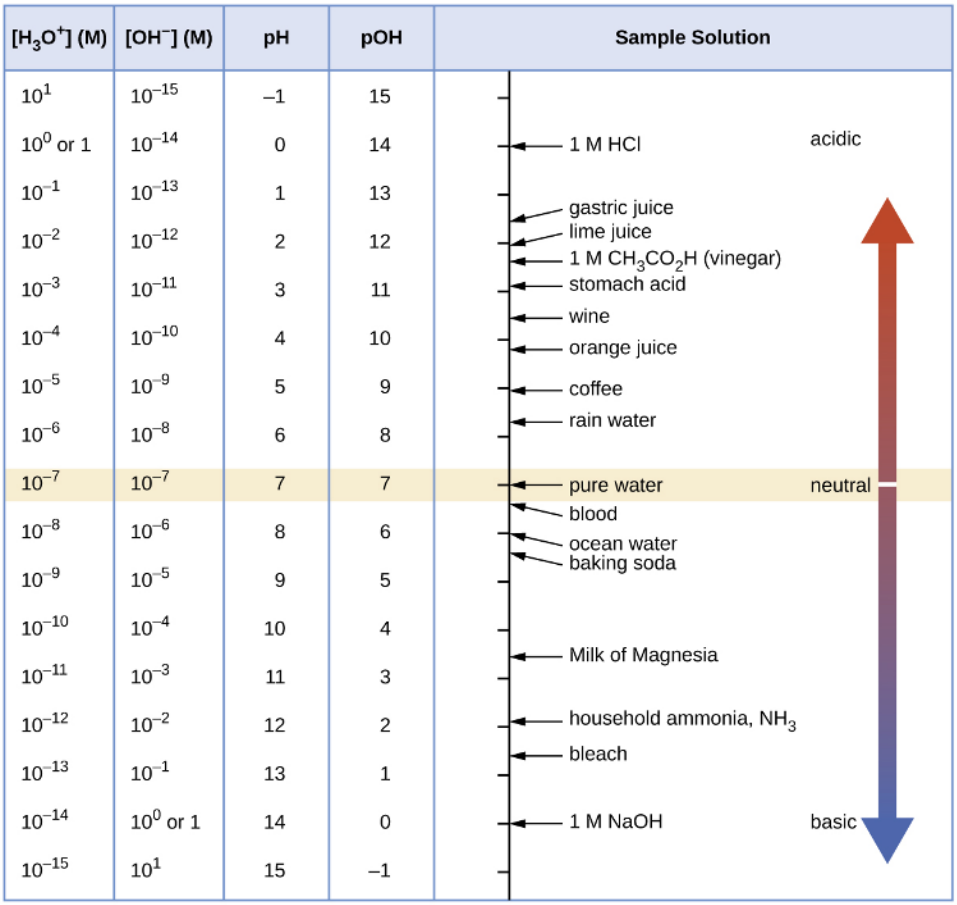


Figure **9.2.1**: The pH and pOH scales represent concentrations of H_3O^+ and OH^-, respectively. The pH and pOH values of some common substances at 25 °C are shown in this chart.

Example 9.2.1: Calculation of pH from $[H_3O^+]$

What is the pH of stomach acid, a solution of HCl with a hydronium ion concentration of $1.2 \times 10^{-3}\ M$?

Solution

$$\begin{aligned} pH &= -\log\left[H_3O^+\right] \\ &= -\log\left(1.2 \times 10^{-3}\right) \\ &= -(-2.92) = 2.92 \end{aligned}$$

(The use of logarithms is explained in Appendix B. When taking the log of a value, keep as many decimal places in the result as there are significant figures in the value.)

Exercise 9.2.1

Water exposed to air contains carbonic acid, H_2CO_3, due to the reaction between carbon dioxide and water:

$$CO_2\,(aq) + H_2O\,(l) \rightleftharpoons H_2CO_3\,(aq)$$

Air-saturated water has a hydronium ion concentration caused by the dissolved CO_2 of 2.0×10^{-6} M, about 20-times larger than that of pure water. Calculate the pH of the solution at 25 °C.

Answer

5.70

Example 9.2.2: Calculation of Hydronium Ion Concentration from pH

Calculate the hydronium ion concentration of blood, the pH of which is 7.3.

Solution

$$\begin{aligned} pH = -\log\left[H_3O^+\right] &= 7.3 \\ \log\left[H_3O^+\right] &= -7.3 \\ \left[H_3O^+\right] &= 10^{-7.3} \end{aligned}$$

or

$$\begin{aligned} \left[H_3O^+\right] &= \text{antilog of } -7.3 \\ &= 5 \times 10^{-8} M \end{aligned}$$

(On a calculator take the antilog, or the "inverse" log, of −7.3, or calculate $10^{-7.3}$.)

Exercise 9.2.2

Calculate the hydronium ion concentration of a solution with a pH of −1.07.

Answer

12 *M*

How Sciences Interconnect: Environmental Science

Normal rainwater has a pH between 5 and 6 due to the presence of dissolved CO_2 which forms carbonic acid:

$$H_2O\,(l) + CO_2\,(g) \longrightarrow H_2CO_3\,(aq)$$
$$H_2CO_3\,(aq) \rightleftharpoons H^+\,(aq) + HCO_3^-\,(aq)$$

Acid rain is rainwater that has a pH of less than 5, due to a variety of nonmetal oxides, including CO_2, SO_2, SO_3, NO, and NO_2 being dissolved in the water and reacting with it to form not only carbonic acid, but sulfuric acid and nitric acid. The formation and subsequent ionization of sulfuric acid are shown here:

$$H_2O(l) + SO_3(g) \longrightarrow H_2SO_4(aq)$$
$$H_2SO_4(aq) \longrightarrow H^+(aq) + HSO_4^-(aq)$$

Carbon dioxide is naturally present in the atmosphere because most organisms produce it as a waste product of metabolism. Carbon dioxide is also formed when fires release carbon stored in vegetation or fossil fuels. Sulfur trioxide in the atmosphere is naturally produced by volcanic activity, but it also originates from burning fossil fuels, which have traces of sulfur, and from the process of "roasting" ores of metal sulfides in metal-refining processes. Oxides of nitrogen are formed in internal combustion engines where the high temperatures make it possible for the nitrogen and oxygen in air to chemically combine.

Acid rain is a particular problem in industrial areas where the products of combustion and smelting are released into the air without being stripped of sulfur and nitrogen oxides. In North America and Europe until the 1980s, it was responsible for the destruction of forests and freshwater lakes, when the acidity of the rain actually killed trees, damaged soil, and made lakes uninhabitable for all but the most acid-tolerant species. Acid rain also corrodes statuary and building facades that are made of marble and limestone (Figure **9.2.2**). Regulations limiting the amount of sulfur and nitrogen oxides that can be released into the atmosphere by industry and automobiles have reduced the severity of acid damage to both natural and manmade environments in North America and Europe. It is now a growing problem in industrial areas of China and India.

For further information on acid rain, visit this website hosted by the US Environmental Protection Agency.



(a) (b)

Figure **9.2.2**: (a) Acid rain makes trees more susceptible to drought and insect infestation, and depletes nutrients in the soil. (b) It also is corrodes statues that are carved from marble or limestone. (credit a: modification of work by Chris M Morris; credit b: modification of work by "Eden, Janine and Jim"/Flickr)

✔ Example ✔ 9.2.3: Calculation of pOH

What are the **pOH** and the \(\text{pH} of a 0.0125-*M* solution of potassium hydroxide, **KOH**?

Solution

Potassium hydroxide is a highly soluble ionic compound and completely dissociates when dissolved in dilute solution, yielding $[OH^-] = 0.0125\ M$:

$$\text{pOH} = -\log[OH^-] = -\log 0.0125$$
$$= -(-1.903) = 1.903$$

The pH can be found from the pOH:

$$\mathrm{pH} + \mathrm{pOH} = 14.00$$
$$pH = 14.00 - pOH$$
$$= 14.00 - 1.903 = 12.10$$

? Exercise 9.2.3

The hydronium ion concentration of vinegar is approximately 4×10^{-3} M. What are the corresponding values of pOH and pH?

Answer

pOH = 11.6, pH = 2.4

The acidity of a solution is typically assessed experimentally by measurement of its pH. The pOH of a solution is not usually measured, as it is easily calculated from an experimentally determined pH value. The pH of a solution can be directly measured using a pH meter (Figure 9.2.3).



Figure 9.2.3: (a) A research-grade pH meter used in a laboratory can have a resolution of 0.001 pH units, an accuracy of ± 0.002 pH units, and may cost in excess of $1000. (b) A portable pH meter has lower resolution (0.01 pH units), lower accuracy (± 0.2 pH units), and a far lower price tag. (credit b: modification of work by Jacopo Werther)

The pH of a solution may also be visually estimated using colored indicators (Figure 9.2.4). The acid-base equilibria that enable use of these indicator dyes for pH measurements are described in a later section of this chapter.



Figure 9.2.4: (a) A solution containing a dye mixture, called universal indicator, takes on different colors depending upon its pH. (b) Convenient test strips, called pH paper, contain embedded indicator dyes that yield pH-dependent color changes on contact with aqueous solutions.(credit: modification of work by Sahar Atwa)

This page titled 9.2: pH and pOH is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **14.2: pH and pOH** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

9.3: Acid-Base Balance

As with electrolytes, correct balance of acids and bases in the body is essential to proper body functioning. Even a slight variance outside of normal can be life-threatening, so it is important to understand normal acid-base values, as well their causes and how to correct them. The kidneys and lungs work together to correct slight imbalances as they occur. As a result, the kidneys compensate for shortcomings of the lungs, and the lungs compensate for shortcomings of the kidneys.

Arterial Blood Gases

Arterial blood gases (ABG) are measured by collecting blood from an artery, rather than a vein, and are most commonly collected via the radial artery. ABGs measure the pH level of the blood, the partial pressure of arterial oxygen (PaO2), the partial pressure of arterial carbon dioxide (PaCO2), the bicarbonate level (HCO3), and the oxygen saturation level (SaO2).



Prior to collecting blood gases, it is important to ensure the patient has appropriate arterial blood flow to the hand. This is done by performing the Allen test. When performing the Allen test, pressure is held on both the radial and ulnar artery below the wrist. Pressure is released from the ulnar artery to check if blood flow is adequate. If arterial blood flow is adequate, warmth and color should return to the hand.

pH

pH is a scale from 0-14 used to determine the acidity or alkalinity of a substance. A neutral pH is 7, which is the same pH as water. Normally, the blood has a pH between 7.35 and 7.45. A blood pH of less than 7.35 is considered acidic, and a blood pH of more than 7.45 is considered alkaline.

The pH of blood is a measure of hydrogen ion concentration. A low pH, less than 3.5, occurs in acidosis when the blood has a high hydrogen ion concentration. A high pH, greater than 7.45, occurs in alkalosis when the blood has a low hydrogen ion concentration. Hydrogen ions are by-products of the metabolism of substances such as proteins, fats, and carbohydrates. These by-products create extra hydrogen ions (H+) in the blood that need to be balanced and kept within normal range as described earlier.

The body has several mechanisms for maintaining blood pH. The lungs are essential for maintaining pH and the kidneys also play a role. For example, when the pH is too low (i.e., during acidosis), the respiratory rate quickly increases to eliminate acid in the form of carbon dioxide (CO2). The kidneys excrete additional hydrogen ions (acid) in the urine and retain bicarbonate (base). Conversely, when the pH is too high (i.e., during alkalosis), the respiratory rate decreases to retain acid in the form of CO2. The kidneys excrete bicarbonate (base) in the urine and retain hydrogen ions (acid).

PaCO2

PaCO2 is the partial pressure of arterial carbon dioxide in the blood. The normal PaCO2 level is 35-45 mmHg. CO2 forms an acid in the blood that is regulated by the lungs by changing the rate or depth of respirations.

As the respiratory rate increases or becomes deeper, additional CO2 is removed causing decreased acid (H+) levels in the blood and increased pH (so the blood becomes more alkaline). As the respiratory rate decreases or becomes more shallow, less CO2 is removed causing increased acid (H+) levels in the blood and decreased pH (so the blood becomes more acidic).

Generally, the lungs work quickly to regulate the PaCO2 levels and cause a quick change in the pH. Therefore, an acid-base problem caused by hypoventilation can be quickly corrected by increasing ventilation, and a problem caused by hyperventilation can be quickly corrected by decreasing ventilation. For example, if an anxious patient is hyperventilating, they may be asked to breathe into a paper bag to rebreathe some of the CO2 they are blowing off. Conversely, a postoperative patient who is experiencing hypoventilation due to the sedative effects of receiving morphine is asked to cough and deep breathe to blow off more CO2.

HCO3

HCO3 is the bicarbonate level of the blood and the normal range is 22-26. HCO3 is a base managed by the kidneys and helps to make the blood more alkaline. The kidneys take longer than the lungs to adjust the acidity or alkalinity of the blood, and the response is not visible upon assessment. As the kidneys sense an alteration in pH, they begin to retain or excrete HCO3, depending on what is needed. If the pH becomes acidic, the kidneys retain HCO3 to increase the amount of bases present in the blood to increase the pH. Conversely, if the pH becomes alkalotic, the kidneys excrete more HCO3, causing the pH to decrease.

PaO2

PaO2 is the partial pressure of arterial oxygen in the blood. It more accurately measures a patient's oxygenation status than SaO2 (the measurement of hemoglobin saturation with oxygen). Therefore, ABG results are also used to manage patients in respiratory distress.

Note

Read more information about interpreting ABG results in the "Oxygen Therapy" chapter in Open RN *Nursing Skills*.

See Table 15.5a for a review of ABG components, normal values, and key critical values. A critical ABG value means there is a greater risk of serious complications and even death if not corrected rapidly. For example, a pH of 7.10, a shift of only 0.25 below normal, is often fatal because this level of acidosis can cause cardiac or respiratory arrest or significant hyperkalemia.[1] As you can see, failure to recognize ABG abnormalities can have serious consequences for your patients.

Table 15.5a ABG Components, Descriptions, Adult Normal Values, and Critical Values[2]

ABG Component	Description	Adult Normal Value	Critical Value
pH	• Acidity (<7.35) or alkalinity (>7.45) of blood. • Measure of H+ ions (acids). • Affected by the lungs via hypo- or hyperventilation or the kidneys through bicarbonate retention.	7.35-7.45	<7.25 >7.60
PaO2	• Pressure of oxygen in the blood.	80-100 mmHg	<60 mmHg
PaCO2	• Pressure of carbon dioxide in the blood. • CO2 is an acid managed by the lungs. • As PaCO2 increases, the blood becomes more acidic and the pH decreases. • As PaCO2 decreases, the blood becomes less acidic and the pH increases.	35-45 mmHg	<25 mmHg >60 mmHg
HCO3	• Bicarbonate level in the blood. • HCO3 is a base managed by the kidneys. • As HCO3 increases, the blood becomes more alkaline and the pH increases. • As HCO3 decreases, the blood becomes more acidic and the pH decreases.	22-26 mEq/L	<10 mEq/L >40 mEq/L
SaO2	• Oxygen saturation in the blood.	95-100%	<88%

Video Review of Acid-Base Balance[3]



Interpreting Arterial Blood Gases

After the ABG results are received, it is important to understand how to interpret them. A variety of respiratory, metabolic, electrolyte, or circulatory problems can cause acid-base imbalances. Correct interpretation also helps the nurse and other health care providers determine the appropriate treatment and evaluate the effectiveness of interventions.

Arterial blood gasses can be interpreted as one of four conditions: respiratory acidosis, respiratory alkalosis, metabolic acidosis, or metabolic alkalosis. Once this interpretation is made, conditions can further be classified as compensated, partially compensated, or uncompensated. A simple way to remember how to interpret ABGs is by using the ROME method of interpretation, which stands for **R**espiratory **O**pposite, **M**etabolic **E**qual. This means that the respiratory component (PaCO2) moves in the opposite direction of the pH if the respiratory system is causing the imbalance. If the metabolic system is causing the imbalance, the metabolic component (HCO3) moves in the same direction as the pH. Some nurses find the Tic-Tac-Toe method of interpretation helpful. If you would like to learn more about this method, click on the hyperlink below to view a video.

Review of Tic-Tac-Toe Method of ABG Interpretation[4]



Respiratory Acidosis

Respiratory acidosis develops when carbon dioxide (CO2) builds up in the body (referred to as **hypercapnia**), causing the blood to become increasingly acidic. Respiratory acidosis is identified when reviewing ABGs and the pH level is below 7.35 and the PaCO2 level is above 45, indicating the cause of the acidosis is respiratory. Note that in respiratory acidosis, as the PaCO2 level increases, the pH level decreases. Respiratory acidosis is typically caused by a medical condition that decreases the exchange of oxygen and carbon dioxide at the alveolar level, such as an acute asthma exacerbation, chronic obstructive pulmonary disease (COPD), or an acute heart failure exacerbation causing pulmonary edema. It can also be caused by decreased ventilation from anesthesia, alcohol, or administration of medications such as opioids and sedatives.

Chronic respiratory diseases, such as COPD, often cause chronic respiratory acidosis that is fully compensated by the kidneys retaining HCO3. Because the carbon dioxide levels build up over time, the body adapts to elevated PaCO2 levels so they are better tolerated. However, in acute respiratory acidosis, the body has not had time to adapt to elevated carbon dioxide levels, causing mental status changes associated with hypercapnia. Acute respiratory acidosis is caused by acute respiratory conditions, such as an asthma attack or heart failure exacerbation with pulmonary edema when the lungs suddenly are not able to ventilate adequately. As breathing slows and respirations become shallow, less CO2 is excreted by the lungs and PaCO2 levels quickly rise.

Signs of symptoms of hypercapnia vary depending upon the level and rate of CO2 accumulation in arterial blood:

- Patients with mild to moderate hypercapnia may be anxious and/or complain of mild dyspnea, daytime sluggishness, headaches, or hypersomnolence.
- Patients with higher levels of CO2 or rapidly developing hypercapnia develop delirium, paranoia, depression, and confusion that can progress to seizures and coma as levels continue to rise.

Individuals with normal lung function typically exhibit a depressed level of consciousness when the PaCO2 is greater than 75 to 80 mmHg, whereas patients with chronic hypercapnia may not develop symptoms until the PaCO2 rises above 90 to 100 mmHg.[5]

When a patient demonstrates signs of potential hypercapnia, the nurse should assess airway, breathing, and circulation. Urgent assistance should be sought, especially if the patient is in respiratory distress. The provider will order an ABG and prescribe treatments based on assessment findings and potential causes. Treatment for respiratory acidosis typically involves improving ventilation and respiration by removing airway restrictions, reversing oversedation, administering nebulizer treatments, or increasing the rate and depth of respiration by using a BiPAP or CPAP devices. BiPAP and CPAP devices provide noninvasive positive pressure ventilation to increase the depth of respirations, remove carbon dioxide, and oxygenate the patient. If these noninvasive interventions are not successful, the patient is intubated and placed on mechanical ventilation.[6],[7]

Note

Read more details about oxygenation equipment in "Oxygen Therapy" in Open RN *Nursing Skills*.

Respiratory Alkalosis

Respiratory alkalosis develops when the body removes too much carbon dioxide through respiration, resulting in increased pH and an alkalotic state. When reviewing ABGs, respiratory alkalosis is identified when pH levels are above 7.45 and the PaCO2 level is below 35. With respiratory alkalosis, notice that as the PaCO2 level decreases, the pH level increases.

Respiratory alkalosis is caused by hyperventilation that can occur due to anxiety, panic attacks, pain, fear, head injuries, or mechanical ventilation. Overdoses of salicylates and other toxins can also cause respiratory alkalosis initially and then often progress to metabolic acidosis in later stages. Acute asthma exacerbations, pulmonary embolisms, or other respiratory disorders can initially cause respiratory alkalosis as the lungs breath faster in an attempt to increase oxygenation, which decreases the PaCO2. After a while, however, these hypoxic disorders cause respiratory acidosis as respiratory muscles tire, breathing slows, and CO2 builds up in the blood.

Patients experiencing respiratory alkalosis often report feelings of shortness of breath, dizziness or light-headedness, chest pain or tightness, paresthesias, and palpitations as a result of decreased carbon dioxide levels.[8] Respiratory alkalosis is not fatal, but it is important to recognize that underlying conditions such as an asthma exacerbation or pulmonary embolism can be life-threatening, so treatment of these underlying conditions is essential. As the pH level increases, the kidneys will attempt to compensate for the shortage of H+ ions by reabsorbing HCO3 before it can be excreted in the urine. This is a slow process, so additional treatment may be necessary.

Treatment of respiratory alkalosis involves treating the underlying cause of the hyperventilation. Acute management of patients who are hyperventilating should focus on patient reassurance, an explanation of the symptoms the patient is experiencing, removal of any stressors, and initiation of breathing retraining. Breathing retraining attempts to focus the patient on abdominal (diaphragmatic) breathing. Read more about breathing retraining in the following box.

Breathing Retraining

While sitting or lying supine, the patient should place one hand on their abdomen and the other on the chest, and then be asked to observe which hand moves with greater excursion. In hyperventilating patients, this will almost always be the hand on the chest. Ask the patient to adjust their breathing so that the hand on the abdomen moves with greater excursion and the hand on the chest barely moves at all. Assure the patient that this is hard to learn and will take some practice to fully master. Ask the patient to breathe in slowly over four seconds, pause for a few seconds, and then breathe out over a period of eight seconds. After 5 to 10 such breathing cycles, the patient should begin to feel a sense of calmness with a reduction in anxiety and an improvement in hyperventilation. Symptoms should ideally resolve with continuation of this breathing exercise.

If the breathing retraining technique is not successful in resolving a hyperventilation episode and severe symptoms persist, the patient may be prescribed a small dose of a short-acting benzodiazepine (e.g., lorazepam 0.5 to 1 mg orally or 0.5 to 1 mg intravenously). Current research indicates that instructing patients who are hyperventilating to rebreathe carbon dioxide (CO2) by

breathing into a paper bag can cause significant hypoxemia with significant complications, so this intervention is no longer recommended. If rebreathing is used, oxygen saturation levels should be continuously monitored.[9]

Metabolic Acidosis

Metabolic acidosis occurs when there is an accumulation of acids (hydrogen ions) and not enough bases (HCO3) in the body. Under normal conditions, the kidneys work to excrete acids through urine and neutralize excess acids by increasing bicarbonate (HCO3) reabsorption from the urine to maintain a normal pH. When the kidneys are not able to perform this buffering function to the level required to excrete and neutralize the excess acid, metabolic acidosis results.

Metabolic acidosis is characterized by a pH level below 7.35 and an HCO3 level below 22 when reviewing ABGs. It is important to notice that both the pH and HCO3 decrease with metabolic acidosis (i.e., the pH and HCO3 move in the same downward direction). A common cause of metabolic acidosis is diabetic ketoacidosis, where acids called ketones build up in the blood when blood sugar is extremely elevated. Another common cause of metabolic acidosis in hospitalized patients is lactic acidosis, which can be caused by impaired tissue oxygenation. Metabolic acidosis can also be caused by increased loss of bicarbonate due to severe diarrhea or from renal disease that causes decreased acid elimination. Additionally, toxins such as salicylate excess can cause metabolic acidosis.[10]

Nurses may first suspect that a patient has metabolic acidosis due to rapid breathing that occurs as the lungs try to remove excess CO2 in an attempt to resolve the acidosis. Other symptoms of metabolic acidosis include confusion, decreased level of consciousness, hypotension, and electrolyte disturbances that can progress to circulatory collapse and death if not treated promptly. It is important to quickly notify the provider of suspected metabolic acidosis so that an ABG can be drawn and treatment prescribed (based on the cause of the metabolic acidosis) to allow acid levels to improve. Treatment includes IV fluids to improve hydration status, glucose management, and circulatory support. When pH drops below 7.1, IV sodium bicarbonate is often prescribed to help neutralize the acids in the blood.[11] [12]

Metabolic Alkalosis

Metabolic alkalosis occurs when there is too much bicarbonate (HCO3) in the body or an excessive loss of acid (H+ ions). Metabolic alkalosis is defined by a pH above 7.45 and an HCO3 level above 26 on ABG results. Note that both pH and HCO3 are elevated in metabolic alkalosis.

Metabolic alkalosis can be caused by gastrointestinal loss of hydrogen ions, excessive urine loss, excessive levels of bicarbonate, or a shift of hydrogen ions from the bloodstream into cells.

Prolonged vomiting or nasogastric suctioning can also cause metabolic alkalosis. Gastric secretions have high levels of hydrogen ions (H+), so as acid is lost, the pH level of the bloodstream increases.

Excessive urinary loss (due to diuretics or excessive mineralocorticoids) can cause metabolic alkalosis due to loss of hydrogen ions in the urine. Intravenous administration of sodium bicarbonate can also cause metabolic alkalosis due to increased levels of bases introduced into the body. Although it was once thought that excessive intake of calcium antacids could cause metabolic alkalosis, it has been found that this only occurs if they are administered concurrently with Kayexelate.[13]

Hydrogen ions may shift into cells due to hypokalemia, causing metabolic alkalosis. When hypokalemia occurs (i.e., low levels of potassium in the bloodstream), potassium shifts out of cells and into the bloodstream in an attempt to maintain a normal level of serum potassium for optimal cardiac function. However, as the potassium (K+) molecules move out of the cells, hydrogen (H+) ions then move into the cells from the bloodstream to maintain electrical neutrality. This transfer of ions causes the pH in the bloodstream to drop, causing metabolic alkalosis.[14]

A nurse may first suspect that a patient has metabolic alkalosis due to a decreased respiratory rate (as the lungs try to retain additional CO2 to increase the acidity of the blood and resolve the alkalosis). The patient may also be confused due to the altered pH level. The nurse should report signs of suspected metabolic alkalosis because uncorrected metabolic alkalosis can result in hypotension and cardiac dysfunction.[15]

Treatment is prescribed based on the ABG results and the suspected cause. For example, treat the cause of the vomiting, stop the gastrointestinal suctioning, or stop the administration of diuretics. If hypokalemia is present, it should be treated. If bicarbonate is being administered, it should be stopped. Patients with kidney disease may require dialysis.[16]

Analyzing ABG Results

Now that we've discussed the differences between the various acid-base imbalances, let's review the steps to systematically interpret ABG results. Table 15.5b outlines the steps of ABG interpretation.

Table 15.5b Analyzing ABG Results[17],[18]

Step	Action
Step 1: pH (normal 7.35-7.45)	If pH is out of range, determine if it is acidosis or alkalosis: • pH <7.35 is acidosis. • pH >7.45 is alkalosis.
Step 2: PaCO2 (normal 35-45 mmHg)	• Is the PaCO2 normal? ◦ PaCO2 <35 is considered alkalotic. ◦ PaCO2 >45 is considered acidotic. • If the PaCO2 is abnormal, determine if this is caused by a respiratory problem. Recall that if the imbalance is caused by a respiratory problem, the PaCO2 moves in the opposite direction of the pH: ◦ If the pH is <7.35 (acidosis) and the PaCO2 is >45 (acidotic), this is respiratory acidosis. ◦ If the pH is >7.45 (alkalosis) and the PaCO2 is <35 (alkalotic), this is respiratory alkalosis. **If the imbalance does not appear to be caused by a respiratory problem, move on to evaluate the HCO3.
Step 3: HCO3 (normal 22-26)	• Is the HCO3 normal? ◦ HCO3 <22 is considered acidotic. ◦ HCO3 >26 is considered alkalotic. • If the HCO3 is abnormal, determine if this caused by a metabolic problem. Recall that the HCO3 moves in the same direction as the pH if the imbalance is caused by a metabolic problem: ◦ If pH is <7.35 (acidosis) and the HCO3 is <22 (acidotic), this is metabolic acidosis. ◦ If the pH is >7.45 (alkalosis) and the HCO3 is >26 (alkalotic), this is metabolic alkalosis.
Step 4: Determine level of compensation	After determining the cause of the pH imbalance, determine if compensation is occurring. • **Fully compensated** = the body has fixed the imbalance by bringing the pH back to normal: ◦ pH is normal (7.35-7.45). ◦ PaCO2 and HCO3 are both out of range. ◦ The cause of the disorder is out of range, and the other value is significantly out of range indicating compensation is occurring. ◦ Recall the respiratory rate quickly compensates for metabolic disorders, and the kidneys take longer to compensate for respiratory disorders. • **Partially compensated** = the body is working to fix the imbalance but hasn't yet brought the pH back to normal: ◦ pH is abnormal (<7.35 or >7.45). ◦ PaCO2 and HCO3 are abnormal. ◦ The CAUSE of the disorder is out of range and the other value is moving out of range, indicating compensation is occurring. • **Uncompensated** = the body is not yet working to bring the pH back to normal: ◦ pH is abnormal (<7.35 or >7.45)

Step	Action
	○ PaCO2 or HCO3 is abnormal, but not both. ○ The CAUSE of the disorder is out of range but the other value is not yet out of range, indicating compensation is not yet occurring.

1. Mitchel, J. H., Wildenthal, K., & Johnson Jr., R. L. (1972). The effects of acid-base disturbances on cardiovascular and pulmonary function. *Kidney International*, *1*, 375-389. https://www.kidney-international.org/article/S0085-2538(15)31047-4/pdf↵
2. WakeMed Pathology Laboratories. (2016). *Critical values*. https://www.wakemed.org/assets/documents/pathology/lab-critical-values.pdf↵
3. Forciea, B. (2017, May 10). *Acid-base balance: Bicarbonate ion buffer*. [Video]. YouTube. All rights reserved. Video used with permission. https://youtu.be/5_S5wZks9v8↵
4. RegisteredNurseRN. (2015, May 6). *ABGs made easy for nurses w/ tic tac toe method for arterial blood gas interpretation*. [Video]. YouTube. All rights reserved. Video used with permission. https://youtu.be/URCS4t9aM5o↵
5. Feller-Kopman, D. J., & Schwartzstein, R. M. (2020). The evaluation, diagnosis, and treatment of the adult patient with acute hypercapnic respiratory failure. *UpToDate*. https://www.uptodate.com/contents/the-evaluation-diagnosis-and-treatment-of-the-adult-patient-with-acute-hypercapnic-respiratory-failure↵
6. A.D.A.M. Medical Encyclopedia [Internet]. Atlanta (GA): A.D.A.M., Inc.; c1997-2021. Respiratory acidosis; [updated 2021, February 8]. https://medlineplus.gov/ency/article/000092.htm↵
7. Feller-Kopman, D. J., & Schwartzstein, R. M. (2020). The evaluation, diagnosis, and treatment of the adult patient with acute hypercapnic respiratory failure. *UpToDate*. https://www.uptodate.com/contents/the-evaluation-diagnosis-and-treatment-of-the-adult-patient-with-acute-hypercapnic-respiratory-failure↵
8. Schwartzstein, R. M., Richards, J., Edlow, J. A., & Roy-Byrne, P. P. (2020). Hyperventilation syndrome in adults. *UpToDate*. https://www.uptodate.com/contents/hyperventilation-syndrome-in-adults↵
9. Schwartzstein, R. M., Richards, J., Edlow, J. A., & Roy-Byrne, P. P. (2020). Hyperventilation syndrome in adults. *UpToDate*. https://www.uptodate.com/contents/hyperventilation-syndrome-in-adults↵
10. Emmett, M., & Szerlip, H. (2020). Approach to the adult with metabolic acidosis. *UpToDate*. https://www.uptodate.com/contents/approach-to-the-adult-with-metabolic-acidosis↵
11. A.D.A.M. Medical Encyclopedia [Internet]. Atlanta (GA): A.D.A.M., Inc.; c1997-2021. Metabolic acidosis; [updated 2021, February 8]. https://medlineplus.gov/ency/article/000335.htm↵
12. Emmett, M., & Szerlip, H. (2020). Approach to the adult with metabolic acidosis. *UpToDate*. https://www.uptodate.com/contents/approach-to-the-adult-with-metabolic-acidosis↵
13. Emmett, M., & Szerlip, H. (2020). Causes of metabolic alkalosis. *UpToDate*. https://www.uptodate.com/contents/causes-of-metabolic-alkalosis↵
14. Emmett, M., & Szerlip, H. (2020). Causes of metabolic alkalosis. *UpToDate*. https://www.uptodate.com/contents/causes-of-metabolic-alkalosis↵
15. This work is a derivative of StatPearls by Brinkman and Sharma and is licensed under CC BY 4.0↵
16. Emmett, M., & Szerlip, H. (2020). Causes of metabolic alkalosis. *UpToDate*. https://www.uptodate.com/contents/causes-of-metabolic-alkalosis↵
17. This work is a derivative of StatPearls by Castro and Keenaghan and is licensed under CC BY 4.0↵
18. Woodruff, D. W. (2012). *6 easy steps to ABG analysis*. Ed4Nurses, Inc. http://www.profcaseyscudmorern.org/uploads/4/5/0/4/45049193/abgebook.pdf↵

This page titled 9.3: Acid-Base Balance is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by Ernstmeyer & Christman (Eds.) (OpenRN) via source content that was edited to the style and standards of the LibreTexts platform.

- **15.5: Acid-Base Balance** by Ernstmeyer & Christman (Eds.) is licensed CC BY 4.0. Original source: https://wtcs.pressbooks.pub/nursingfundamentals.

9.4: Case Study- Navigating the Delicate pH Spectrum in Intensive Care

Introduction: In the intricate dance of bodily functions, acids and bases emerge as pivotal elements, and their balance is crucial for life. This case study reflects on the acute attention to acid-base homeostasis in clinical settings, focusing on the vigilant care nurses provide in maintaining the health of their patients.

Scenario: Lisa, a dedicated nurse in the intensive care unit of Central Hospital, is attentively overseeing the treatment of James, a patient with diabetic ketoacidosis. This condition has caused an unsafe rise in James's blood acidity. Lisa's understanding of the nuanced properties of acids and bases is not just academic; it is knowledge she applies every minute at James's bedside, ensuring his blood pH stays within the narrow range that sustains life.

Understanding Acids and Bases: For Lisa, acids are more than just substances that taste sour or corrode metals; they are the molecules that release hydrogen ions in James's bloodstream, tipping the pH scale towards a potentially dangerous level. Bases, the substances that could help neutralize the excess acidity, are the counterbalance necessary to bring James's pH back to a safer number.

Case Study Questions:

1. **Define acids and bases in terms of their properties.**
2. **How does acid-base balance impact patient health?**

Hands-On Classroom Activities:

1. **pH Testing:** In the "pH Testing" activity, students will utilize pH indicators to determine the acidity or alkalinity of common household substances, followed by a discussion on how the pH levels of these substances could potentially impact human health.

Conclusion: In the intimate setting of the ICU, where each patient's story unfolds with a unique medical challenge, the principles of acid–base chemistry become deeply personal. Nurses like Lisa embody the bridge between theory and practice, applying their understanding of acids and bases to make critical decisions that impact patient health profoundly. This case study showcases the human side of chemical knowledge, where pH levels are more than figures on paper: they are indicators of a patient's journey through illness and recovery, navigated by the careful watch of healthcare professionals.

9.4: Case Study- Navigating the Delicate pH Spectrum in Intensive Care is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

9.E: Exercises

Multiple-choice problems

1. What is the definition of a Brønsted-Lowry acid?
    a. A proton donor
    b. A proton acceptor
    c. An electron pair donor
    d. An electron pair acceptor
2. Which of the following molecules is a base?
    a. HCl
    b. H_2SO_4
    c. NH_3
    d. CH_3COOH
3. What is the conjugate base of HF?
    a. H_2F^+
    b. HF
    c. H_3O^+
    d. F^-
4. What is the conjugate acid of NH_3?
    a. NH_4^+
    b. NH_3
    c. NH_2^-
    d. OH^-
5. What pH does an acidic solution have?
    a. pH < 7
    b. pH = 7
    c. pH > 7
    d. The definition of acidity depends on the molecule.
6. What is an example of an everyday base?
    a. Vinegar
    b. Coffee
    c. Blood
    d. Gastric juice
7. What is the pH of a solution with $[H_3O^+] = 4.1 \times 10^{-5}$ M?
    a. 4.10
    b. 4.39
    c. 5.00
    d. 9.61
8. What is the pOH of a solution with $[H_3O^+] = 1.6 \times 10^{-8}$ M?
    a. 1.60
    b. 6.20
    c. 7.80
    d. 8.00
9. What is the hydronium concentration in a solution whose pH is 4.82?
    a. 6.6×10^5 M
    b. 4.82 M

c. 1.5×10^{-5} M
d. 6.6×10^{-10} M

10. What is the hydroxide concentration in a solution whose pOH is 1.75?
    a. 56 M
    b. 1.75 M
    c. 1.8×10^{-2} M
    d. 5.6×10^{-13} M

Warm-up Problems

1. Calculate the pH and the pOH of each of the following solutions at 25 °C for which the substances ionize completely:
    a. 2.59×10^{-4} M $HClO_4$
    b. 0.21 M NaOH
2. Calculate the pH and the pOH of each of the following solutions at 25 °C for which the substances ionize completely:
    a. 7.1×10^{-5} M $Ba(OH)_2$
    b. 2.5 M KOH
3. Calculate the pH and the pOH of each of the following solutions at 25 °C for which the substances ionize completely:
    a. 0.200 M HCl
    b. 0.0143 M NaOH
4. Calculate the pH and the pOH of each of the following solutions at 25 °C for which the substances ionize completely:
    a. 3.0 M HNO_3
    b. 0.0031 M $Ca(OH)_2$
5. What is the hydronium ion concentration in a solution whose pH is 6.52?
6. What is the hydroxide concentration in a solution whose pOH is 3.81?
7. The hydronium ion concentration in a sample of rainwater is 1.7×10^{-6} M at 25 °C. What is the concentration of hydroxide ions in the rainwater?
8. The hydroxide concentration in household ammonia is 3.2×10^{-3} M at 25 °C. What is the concentration of hydronium ions in the solution?

Problems

1. The ionization constant for water (K_W) is 2.9×10^{-14} at 40 °C. Calculate $[H_3O^+]$, $[OH^-]$, pH, and pOH for pure water at this temperature.
2. The ionization constant for water (K_W) is 9.311×10^{-14} at 60 °C. Calculate $[H_3O^+]$, $[OH^-]$, pH, and pOH for pure water at this temperature.
3. Explain the difference between a weak acid and a strong acid. Provide two examples of each.
4. Explain the difference between a weak base and a strong base. Provide two examples of each.
5. What is the conjugate base of HF?
6. What is the conjugate acid of NH_3?
7. What is conjugate acid of bicarbonate? What is the conjugate base of bicarbonate?
8. What is the conjugate acid of hydrogen phosphate? What is the conjugate base of hydrogen phosphate?

Challenge

- Write the products of the acid-base reaction that occurs between acetic acid and the base methylamine (CH_3NH_2). Identify the conjugate base of acetic acid and the conjugate acid of methylamine.
- The typical pH of blood is 7.40. At this pH, is your blood acidic, basic, or neutral? Calculate the concentration of hydroxide ions present in a sample of normal blood. In addition, determine the number of hydroxide ions in a 1.00 L sample of blood with a pH of 7.40.

Health-Related Questions

1. “Acidosis” occurs when the pH of blood is < 7.35. If a patient has a blood pH of 7.30, what is the concentration of hydroxide and hydronium in their blood?
2. “Alkalosis” occurs when the pH of blood is > 7.45. If a patient has a blood pH of 7.50, what is the concentration of hydroxide and hydronium in their blood?

9.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

10: Introduction to Organic Chemistry

10.1: Drawing organic structures

10.2: Alkanes and isomers

10.3: Functional groups

10.4: Case Study- The Molecular Tapestry of Healing

10.5: 3D Printing Activity- Cyclohexane

10.E: Exercises

10: Introduction to Organic Chemistry is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

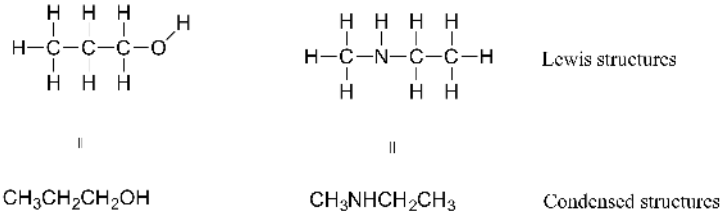
10.1: Drawing organic structures

32

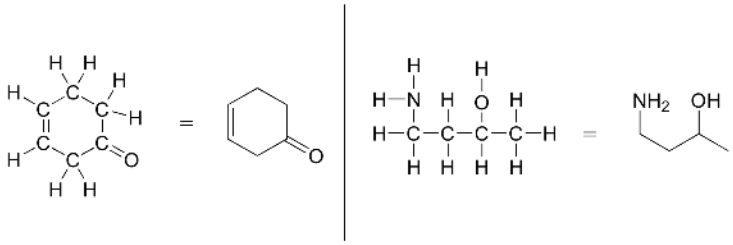
Harper College Chemistry Department

Using the ‘line structure’ convention

If you look ahead at the way organic compounds are drawn in following chapters, you will see that the figures are somewhat different from the Lewis structures you are used to seeing in previous chapters. In some cases, you will see **condensed structures** for smaller molecules instead of full Lewis structures, such as these:



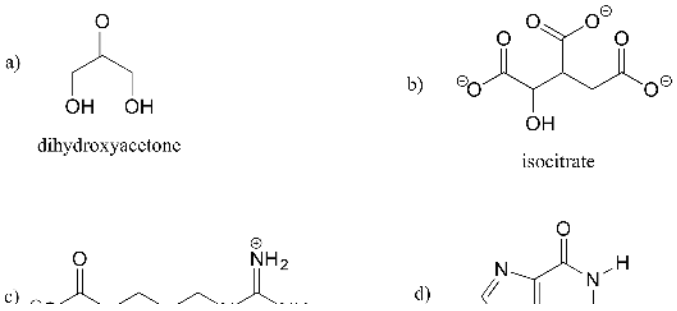
More commonly, organic and biological chemists use an abbreviated drawing convention called **line structures**. The convention is quite simple and makes it easier to draw molecules, but line structures do take a little bit of getting used to. Carbon atoms are depicted not by a capital C, but by a ‘corner’ between two bonds or a free end of a bond. Open-chain molecules are usually drawn out in a ‘zig-zig’ shape. Hydrogens attached to carbons are generally not shown: rather, like lone pairs, they are simply implied (unless a positive formal charge is shown, all carbons are assumed to have a full octet of valence electrons). Hydrogens bonded to nitrogen, oxygen, sulfur, or anything other than carbon *are* shown, but are usually drawn without showing the bond. The following examples illustrate the convention.



As you can see, the ‘pared down’ line structure makes it much easier to see the basic structure of the molecule and the locations where there is something other than C-C and C-H single bonds. For larger, more complex biological molecules, it becomes impractical to use full Lewis structures. Conversely, very small molecules such as ethane should be drawn with their full Lewis or condensed structures.

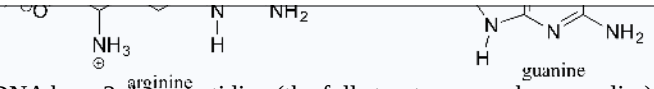
Sometimes, one or more carbon atoms in a line structure will be depicted with a capital C, if doing so makes an explanation easier to follow. *If you label a carbon with a C, you also must draw in the hydrogens for that carbon.*

A good way to test your understanding of the line structure convention is to determine the number of hydrogen atoms in a molecule from its line structure. Do this for the structures below.



https://chem.libretexts.org/@go/page/465664

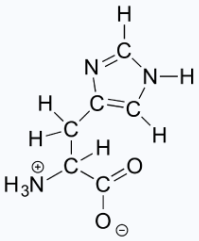
Check Your Learning



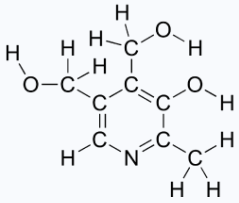
Example 1

a) Draw a line structure for the DNA base 2-deoxycytidine (the full structure was shown earlier)

b) Draw line structures for histidine (an amino acid) and pyridoxine (Vitamin B_6).



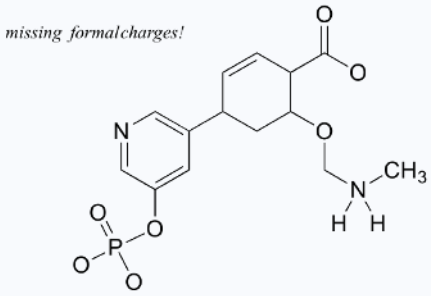
histidine



pyridoxine
(Vitamin B_6)

Example 2

Add non-zero formal charges to the structural drawing below:



Example 3

Find, anywhere in this textbook, one example of each of the common bonding patterns specified below. Check your answers with your instructor or tutor.

a) carbon with one double bond, two single bonds, no lone pairs, and zero formal charge

b) oxygen with two single bonds, two lone pairs, and zero formal charge

c) oxygen with one double bond, two lone pairs, and zero formal charge

d) nitrogen with one double bond, two single bonds, and a +1 formal charge

e) oxygen with one single bond, three lone pairs, and a negative formal charge

10.1: Drawing organic structures is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

10.2: Alkanes and isomers

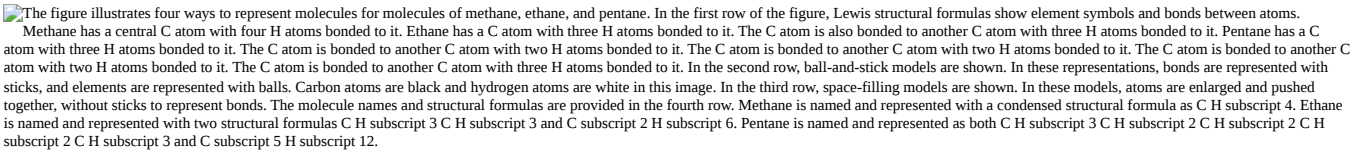
33

Harper College Chemistry Department

Alkanes

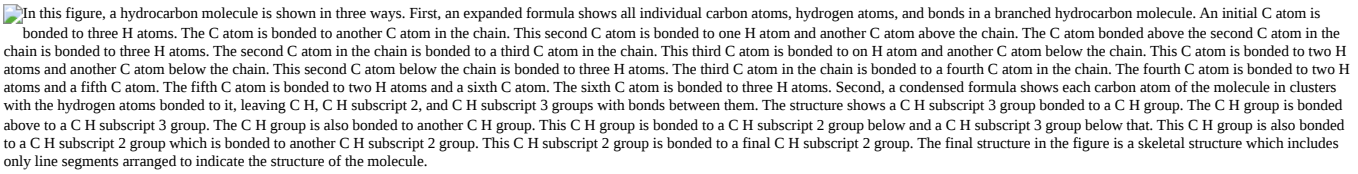
Alkanes, or saturated hydrocarbons, contain only single covalent bonds between carbon atoms. Each of the carbon atoms in an alkane has sp^3 hybrid orbitals and is bonded to four other atoms, each of which is either carbon or hydrogen. The Lewis structures and models of methane, ethane, and pentane are illustrated in Figure 1. Carbon chains are usually drawn as straight lines in Lewis structures, but one has to remember that Lewis structures are not intended to indicate the geometry of molecules. Notice that the carbon atoms in the structural models (the ball-and-stick and space-filling models) of the pentane molecule do not lie in a straight line. Because of the sp^3 hybridization, the bond angles in carbon chains are close to 109.5°, giving such chains in an alkane a zigzag shape.

The structures of alkanes and other organic molecules may also be represented in a less detailed manner by condensed structural formulas (or simply, *condensed formulas*). Instead of the usual format for chemical formulas in which each element symbol appears just once, a condensed formula is written to suggest the bonding in the molecule. These formulas have the appearance of a Lewis structure from which most or all of the bond symbols have been removed. Condensed structural formulas for ethane and pentane are shown at the bottom of Figure 1, and several additional examples are provided in the exercises at the end of this chapter.


The figure illustrates four ways to represent molecules for molecules of methane, ethane, and pentane. In the first row of the figure, Lewis structural formulas show element symbols and bonds between atoms. Methane has a central C atom with four H atoms bonded to it. Ethane has a C atom with three H atoms bonded to it. The C atom is also bonded to another C atom with three H atoms bonded to it. Pentane has a C atom with three H atoms bonded to it. The C atom is bonded to another C atom with two H atoms bonded to it. The C atom is bonded to another C atom with two H atoms bonded to it. The C atom is bonded to another C atom with two H atoms bonded to it. The C atom is bonded to another C atom with three H atoms bonded to it. In the second row, ball-and-stick models are shown. In these representations, bonds are represented with sticks, and elements are represented with balls. Carbon atoms are black and hydrogen atoms are white in this image. In the third row, space-filling models are shown. In these models, atoms are enlarged and pushed together, without sticks to represent bonds. The molecule names and structural formulas are provided in the fourth row. Methane is named and represented with a condensed structural formula as C H subscript 4. Ethane is named and represented with two structural formulas C H subscript 3 C H subscript 3 and C subscript 2 H subscript 6. Pentane is named and represented as both C H subscript 3 C H subscript 2 C H subscript 2 C H subscript 2 C H subscript 3 and C subscript 5 H subscript 12.

Pictured are the Lewis structures, ball-and-stick models, and space-filling models for molecules of methane, ethane, and pentane.

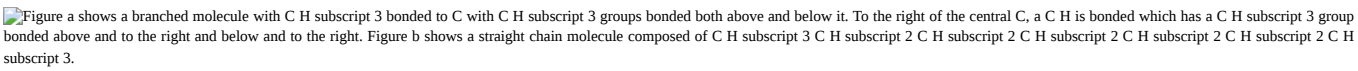
A common method used by organic chemists to simplify the drawings of larger molecules is to use a skeletal structure (also called a line-angle structure). In this type of structure, carbon atoms are not symbolized with a C, but represented by each end of a line or bend in a line. Hydrogen atoms are not drawn if they are attached to a carbon. Other atoms besides carbon and hydrogen are represented by their elemental symbols. Figure 2 shows three different ways to draw the same structure.


In this figure, a hydrocarbon molecule is shown in three ways. First, an expanded formula shows all individual carbon atoms, hydrogen atoms, and bonds in a branched hydrocarbon molecule. An initial C atom is bonded to three H atoms. The C atom is bonded to another C atom in the chain. This second C atom is bonded to one H atom and another C atom above the chain. The C atom bonded above the second C atom in the chain is bonded to three H atoms. The second C atom in the chain is bonded to a third C atom in the chain. This third C atom is bonded to on H atom and another C atom below the chain. This C atom is bonded to two H atoms and another C atom below the chain. This second C atom below the chain is bonded to three H atoms. The third C atom in the chain is bonded to a fourth C atom in the chain. The fourth C atom is bonded to two H atoms and a fifth C atom. The fifth C atom is bonded to two H atoms and a sixth C atom. The sixth C atom is bonded to three H atoms. Second, a condensed formula shows each carbon atom of the molecule in clusters with the hydrogen atoms bonded to it, leaving C H, C H subscript 2, and C H subscript 3 groups with bonds between them. The structure shows a C H subscript 3 group bonded to a C H group. The C H group is bonded above to a C H subscript 3 group. The C H group is also bonded to another C H group. This C H group is bonded to a C H subscript 2 group below and a C H subscript 3 group below that. This C H group is also bonded to a C H subscript 2 group which is bonded to another C H subscript 2 group. This C H subscript 2 group is bonded to a final C H subscript 2 group. The final structure in the figure is a skeletal structure which includes only line segments arranged to indicate the structure of the molecule.

The same structure can be represented three different ways: an expanded formula, a condensed formula, and a skeletal structure.

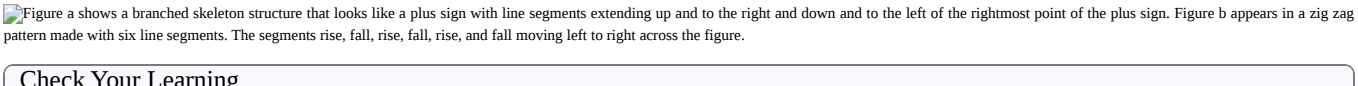
Drawing Skeletal Structures

Draw the skeletal structures for these two molecules:


Figure a shows a branched molecule with C H subscript 3 bonded to C with C H subscript 3 groups bonded both above and below it. To the right of the central C, a C H is bonded which has a C H subscript 3 group bonded above and to the right and below and to the right. Figure b shows a straight chain molecule composed of C H subscript 3 C H subscript 2 C H subscript 2 C H subscript 2 C H subscript 2 C H subscript 2 C H subscript 3.

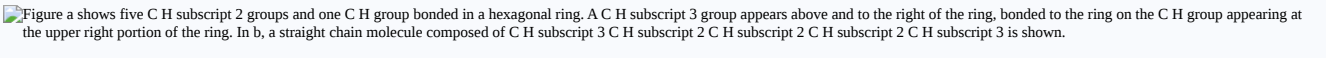
Solution

Each carbon atom is converted into the end of a line or the place where lines intersect. All hydrogen atoms attached to the carbon atoms are left out of the structure (although we still need to recognize they are there):


Figure a shows a branched skeleton structure that looks like a plus sign with line segments extending up and to the right and down and to the left of the rightmost point of the plus sign. Figure b appears in a zig zag pattern made with six line segments. The segments rise, fall, rise, fall, rise, and fall moving left to right across the figure.

Check Your Learning

Draw the skeletal structures for these two molecules:

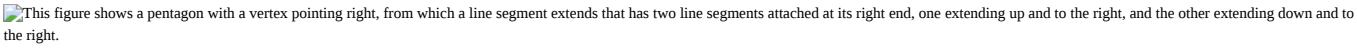

Figure a shows five C H subscript 2 groups and one C H group bonded in a hexagonal ring. A C H subscript 3 group appears above and to the right of the ring, bonded to the ring on the C H group appearing at the upper right portion of the ring. In b, a straight chain molecule composed of C H subscript 3 C H subscript 2 C H subscript 2 C H subscript 2 C H subscript 3 is shown.

Answer:


In a, a hexagon with a vertex at the top is shown. The vertex just to the right has a line segment attached that extends up and to the right. In b, a zig zag pattern is shown in which line segments rise, fall, rise, fall, and rise moving left to right.

Interpreting Skeletal Structures

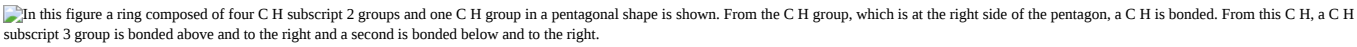
Identify the chemical formula (empirical formula) of the molecule represented here:


This figure shows a pentagon with a vertex pointing right, from which a line segment extends that has two line segments attached at its right end, one extending up and to the right, and the other extending down and to the right.

Solution

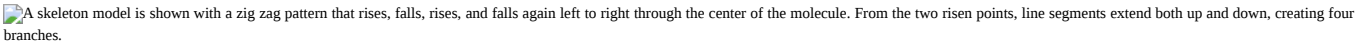
There are eight places where lines intersect or end, meaning that there are eight carbon atoms in the molecule. Since we know that carbon atoms tend to make four bonds, each carbon atom will have the number of hydrogen atoms that are required for four bonds to obey the octet rule. This compound contains 16 hydrogen atoms for a molecular formula of C_8H_{16}.

Location of the hydrogen atoms:


In this figure a ring composed of four C H subscript 2 groups and one C H group in a pentagonal shape is shown. From the C H group, which is at the right side of the pentagon, a C H is bonded. From this C H, a C H subscript 3 group is bonded above and to the right and a second is bonded below and to the right.

Check Your Learning

Identify the chemical formula of the molecule represented here:


A skeleton model is shown with a zig zag pattern that rises, falls, rises, and falls again left to right through the center of the molecule. From the two risen points, line segments extend both up and down, creating four branches.

Answer:

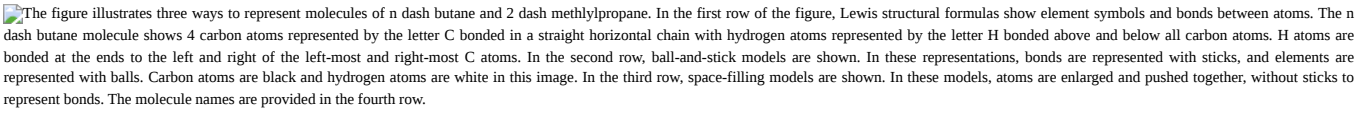
C_9H_{20}

All alkanes are composed of carbon and hydrogen atoms and have similar bonds, structures, and formulas; noncyclic alkanes all have a formula of C_nH_{2n+2}. The number of carbon atoms present in an alkane has no limit. Greater numbers of atoms in the molecules will lead to stronger intermolecular attractions (dispersion forces) and correspondingly different physical properties of the molecules. Properties such as melting point and boiling point (Table 1) usually change smoothly and predictably as the number of carbon and hydrogen atoms in the molecules change.

Properties of Some Alkanes[3]

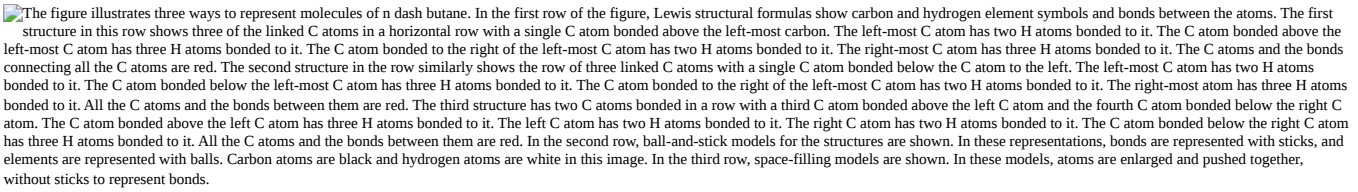
Alkane	Molecular Formula	Melting Point (°C)	Boiling Point (°C)	Phase at STP[4]	Number of Structural Isomers
methane	CH_4	–182.5	–161.5	gas	1
ethane	C_2H_6	–183.3	–88.6	gas	1
propane	C_3H_8	–187.7	–42.1	gas	1
butane	C_4H_{10}	–138.3	–0.5	gas	2
pentane	C_5H_{12}	–129.7	36.1	liquid	3
hexane	C_6H_{14}	–95.3	68.7	liquid	5
heptane	C_7H_{16}	–90.6	98.4	liquid	9
octane	C_8H_{18}	–56.8	125.7	liquid	18
nonane	C_9H_{20}	–53.6	150.8	liquid	35
decane	$C_{10}H_{22}$	–29.7	174.0	liquid	75
tetradecane	$C_{14}H_{30}$	5.9	253.5	solid	1858
octadecane	$C_{18}H_{38}$	28.2	316.1	solid	60,523

Hydrocarbons with the same formula, including alkanes, can have different structures. For example, two alkanes have the formula C_4H_{10}: They are called *n*-butane and 2-methylpropane (or isobutane), and have the following Lewis structures:


The figure illustrates three ways to represent molecules of n dash butane and 2 dash methlylpropane. In the first row of the figure, Lewis structural formulas show element symbols and bonds between atoms. The n dash butane molecule shows 4 carbon atoms represented by the letter C bonded in a straight horizontal chain with hydrogen atoms represented by the letter H bonded above and below all carbon atoms. H atoms are bonded at the ends to the left and right of the left-most and right-most C atoms. In the second row, ball-and-stick models are shown. In these representations, bonds are represented with sticks, and elements are represented with balls. Carbon atoms are black and hydrogen atoms are white in this image. In the third row, space-filling models are shown. In these models, atoms are enlarged and pushed together, without sticks to represent bonds. The molecule names are provided in the fourth row.

The compounds *n*-butane and 2-methylpropane are structural isomers (the term constitutional isomers is also commonly used). Constitutional isomers have the same molecular formula but different bonding arrangements of the atoms in their molecules. The *n*-butane molecule contains an *unbranched chain*, meaning that no carbon atom is bonded to more than two other carbon atoms. We use the term *normal*, or the prefix *n*, to refer to a chain of carbon atoms without branching. The compound 2–methylpropane has a branched chain (the carbon atom in the center of the Lewis structure is bonded to three other carbon atoms)

Identifying isomers from Lewis structures is not as easy as it looks. Lewis structures that look different may actually represent the same isomers. For example, the three structures in Figure 3 all represent the same molecule, *n*-butane, and hence are not different isomers. They are identical because each contains an unbranched chain of four carbon atoms.


The figure illustrates three ways to represent molecules of n dash butane. In the first row of the figure, Lewis structural formulas show carbon and hydrogen element symbols and bonds between the atoms. The first structure in this row shows three of the linked C atoms in a horizontal row with a single C atom bonded above the left-most carbon. The left-most C atom has two H atoms bonded to it. The C atom bonded above the left-most C atom has three H atoms bonded to it. The C atom bonded to the right of the left-most C atom has two H atoms bonded to it. The right-most C atom has three H atoms bonded to it. The C atoms and the bonds connecting all the C atoms are red. The second structure in the row similarly shows the row of three linked C atoms with a single C atom bonded below the C atom to the left. The left-most C atom has two H atoms bonded to it. The C atom bonded below the left-most C atom has three H atoms bonded to it. The C atom bonded to the right of the left-most C atom has two H atoms bonded to it. The right-most atom has three H atoms bonded to it. All the C atoms and the bonds between them are red. The third structure has two C atoms bonded in a row with a third C atom bonded above the left C atom and the fourth C atom bonded below the right C atom. The C atom bonded above the left C atom has three H atoms bonded to it. The left C atom has two H atoms bonded to it. The right C atom has two H atoms bonded to it. The C atom bonded below the right C atom has three H atoms bonded to it. All the C atoms and the bonds between them are red. In the second row, ball-and-stick models for the structures are shown. In these representations, bonds are represented with sticks, and elements are represented with balls. Carbon atoms are black and hydrogen atoms are white in this image. In the third row, space-filling models are shown. In these models, atoms are enlarged and pushed together, without sticks to represent bonds.

> These three representations of the structure of n-butane are not isomers because they all contain the same arrangement of atoms and bonds.

10.2: Alkanes and isomers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

10.3: Functional groups

34

Harper College Chemistry Department

Adapted from LibreTexts: Organic Chemistry With a Biological Emphasis by Tim Soderberg (University of Minnesota, Morris) 1.2: Functional Groups and Organic nomenclature

Functional groups in organic compounds

Functional groups are structural units within organic compounds that are defined by specific bonding arrangements between specific atoms. The structure of capsaicin (Figure 1) incorporates several functional groups, labeled in the figure below and explained throughout this section.

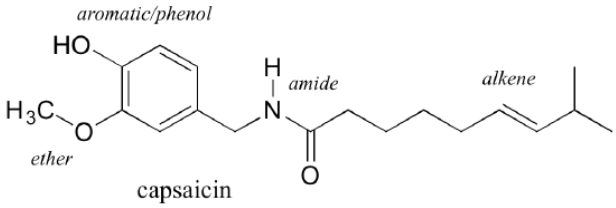
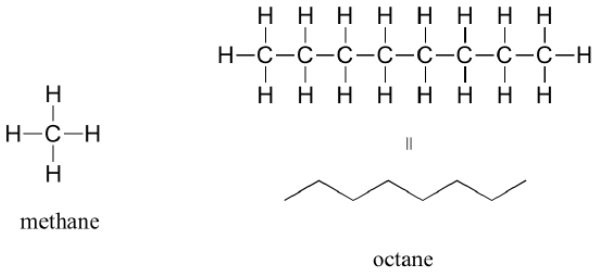


Figure 1. Structure of capsaicin with labeled functional groups.

As we progress in our study of organic chemistry, it will become extremely important to be able to quickly recognize the most common functional groups, because *they are the key structural elements that define how organic molecules react*. For now, we will only worry about drawing and recognizing each functional group, as depicted by Lewis and line structures.

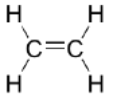
The 'default' in organic chemistry (essentially, the *lack* of any functional groups) is given the term **alkane**, characterized by single bonds between carbon and carbon, or between carbon and hydrogen. Methane, CH_4, is the natural gas you may burn in your furnace. Octane, C_8H_{18}, is a component of gasoline.

Alkanes

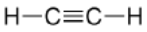


Alkenes (sometimes called **olefins**) have carbon-carbon double bonds, and **alkynes** have carbon-carbon triple bonds. Ethene, the simplest alkene example, is a gas that serves as a cellular signal in fruits to stimulate ripening. If you want bananas to ripen quickly, put them in a paper bag along with an apple – the apple emits ethene gas, setting off the ripening process in the bananas. Ethyne, commonly called acetylene, is used as a fuel in welding blow torches.

Alkenes and alkynes

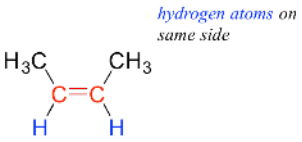


ethene
(an alkene)



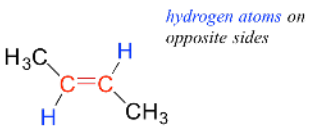
ethyne
(an alkyne)

The bonding nature in alkenes is trigonal planar and in alkynes is linear. Furthermore, many alkenes can take two geometric forms: ***cis*** or ***trans***. The *cis* and *trans* forms of a given alkene are different molecules with different physical properties because there is a very high energy barrier to rotation about a double bond. In the example below, the difference between *cis* and *trans* alkenes is readily apparent.





cis-alkene



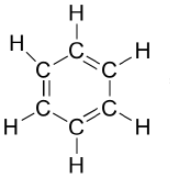


trans-alkene

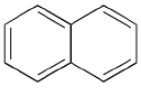
Alkanes, alkenes, and alkynes are all classified as **hydrocarbons**, because they are composed solely of carbon and hydrogen atoms. Alkanes are said to be **saturated hydrocarbons**, because the carbons are bonded to the maximum possible number of hydrogens – in other words, they are *saturated* with hydrogen atoms. The double and triple-bonded carbons in alkenes and alkynes have fewer hydrogen atoms bonded to them – they are thus referred to as **unsaturated hydrocarbons**. Hydrogen can be added to double and triple bonds, in a type of reaction called 'hydrogenation,' which will be discussed in a later chapter.

The **aromatic** group is exemplified by benzene (which used to be a commonly used solvent in the organic lab, but was shown to be carcinogenic later), and naphthalene, a compound with a distinctive 'mothball' smell. Aromatic groups are planar (flat) ring structures and are widespread in nature.

Aromatics

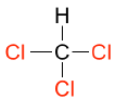


benzene

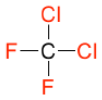


napthalene

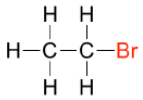
When the carbon of an alkane is bonded to one or more halogens, the group is referred to as a **alkyl halide** or **haloalkane**. Chloroform is a useful solvent in the laboratory and was one of the earlier anesthetics used in surgery. Chlorodifluoromethane was used as a refrigerant and a propellant in aerosol sprays until the late twentieth century; but its use was discontinued after it was found to have harmful effects on the ozone layer. Bromoethane is a simple alkyl halide often used in organic synthesis. Alkyl halides groups are quite rare in biomolecules.



trichloromethane
(chloroform)



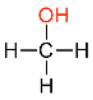
dichlorodifluoromethane
(Freon-12)



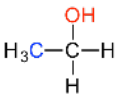
bromoethane

Haloalkanes

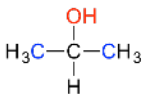
In the **alcohol** functional group, a single-bonded carbon is bonded to an OH group (the OH group, by itself, is referred to as a **hydroxyl**) not to be confused with the hydroxide polyatomic ion, OH^-. Except for methanol, all alcohols can be classified as primary, secondary, or tertiary. In a **primary alcohol**, the carbon bonded to the hydroxyl group is also bonded to only one other carbon. In a **secondary alcohol** and **tertiary alcohol,** the carbon is bonded to two or three other carbons, respectively. When the hydroxyl group is *directly* attached to an aromatic ring, the resulting group is called a **phenol**. The sulfur analog of an alcohol is called a **thiol** (from the Greek *thio*, for sulfur).



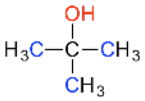
methanol



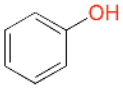
primary alcohol



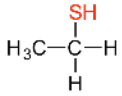
secondary alcohol



tertiary alcohol



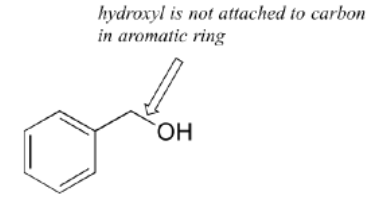
phenol



thiol

Alcohols, phenols, and thiols

Note that the definition of a phenol states that the hydroxyl oxygen must be *directly* attached to one of the carbons of the aromatic ring. The compound below, therefore, is *not* a phenol – it is a primary alcohol.

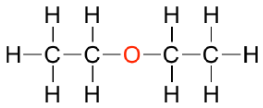


primary alcohol
(*not* a phenol)

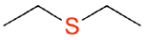
The distinction is important, as there is a significant difference in the reactivity of alcohols and phenols.

In an **ether** functional group, a central oxygen is bonded to two carbons. Below is the structure of diethyl ether, a common laboratory solvent and also one of the first compounds to be used as an anesthetic during operations. The sulfur analog of an ether is called a **thioether** or **sulfide**.

Ethers and sulfides



an ether



a sulfide

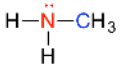
Amines are characterized by nitrogen atoms with single bonds to hydrogen and carbon. Just as there are primary, secondary and tertiary alcohols, there are primary, secondary and tertiary amines. Ammonia is a special case with no carbon atoms, only hydrogen.

One of the most important properties of amines is that they are basic and are readily protonated to form **ammonium** cations. In the case where a nitrogen has four bonds to carbon (which is somewhat unusual in biomolecules), it is called a quaternary ammonium ion.

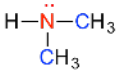
Amines



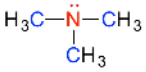
ammonia



a primary amine



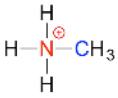
a secondary amine



a tertiary amine



ammonium ion

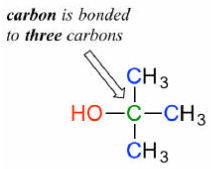


a primary ammonium ion

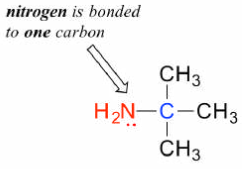


a quaternary ammonium ion

Note: Do not be confused by how the terms, ‘primary’, ‘secondary’, and ‘tertiary’ are applied to alcohols and amines – the definitions are different. In alcohols, what matters is how many other carbons the alcohol *carbon* is bonded to, while in amines, what matters is how many carbons the *nitrogen* is bonded to.



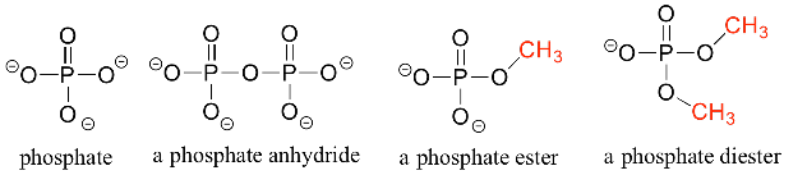
a *tertiary* alcohol



a *primary* amine

Phosphate and its derivative functional groups are ubiquitous in biomolecules. A phosphate linked to a single organic group is called a **phosphate ester**; when it has links to two organic groups it is called a **phosphate diester**. A linkage between two phosphates creates a **phosphate anhydride**.

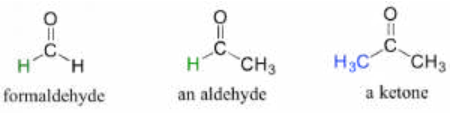
Organic phosphates



There are a number of functional groups that contain a carbon-oxygen double bond, which is commonly referred to as a **carbonyl**. Ketones and aldehydes are two closely related carbonyl-based functional groups that react in very similar ways. In a **ketone**, the carbon atom of a carbonyl is bonded to two other carbons. In an **aldehyde**, the carbonyl carbon is bonded on one side to a hydrogen, and on the other side to a carbon. The exception to this definition is formaldehyde, in which the carbonyl carbon has bonds to two hydrogens.

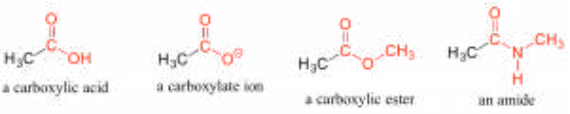
A group with a carbon-nitrogen double bond is called an **imine**, or sometimes a **Schiff base.**

Aldehydes, ketones, and imines

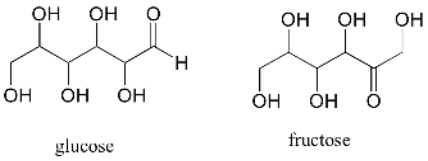


When a carbonyl carbon is bonded on one side to a carbon (or hydrogen) and on the other side to an oxygen, nitrogen, or sulfur, the functional group is considered to be one of the '**carboxylic acid derivatives**', a designation that describes a set of related functional groups. The eponymous member of this family is the **carboxylic acid** functional group, in which the carbonyl is bonded to a hydroxyl group. The conjugate base of a carboxylic acid is a **carboxylate**. Other derivatives are carboxylic esters (usually just called **'esters'**) and **amides,** to name a few. These carboxylic acid derivatives are very common in biological molecules and metabolic pathways.

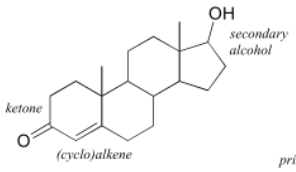
Carboxylic acid derivatives



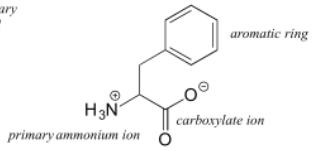
A single compound often contains several functional groups, particularly in biological organic chemistry. The six-carbon sugar molecules glucose and fructose, for example, contain aldehyde and ketone groups, respectively, and both contain five alcohol groups (a compound with several alcohol groups is often referred to as a ' **polyol'**).



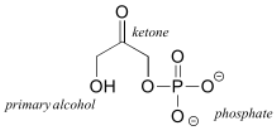
The hormone testosterone, the amino acid phenylalanine, and the glycolysis metabolite dihydroxyacetone phosphate all contain multiple functional groups, as labeled below.



testosterone



phenylalanine



dihydroxyacetone phosphate (DHAP)

While not in any way a complete list, this section has covered most of the important functional groups that we will encounter in biological organic chemistry.

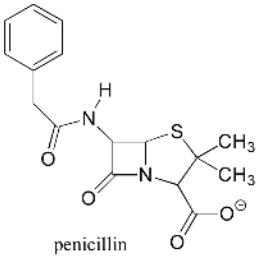
The table here summarizes the structures discussed in this chapter:

This table provides compound names, structures with functional groups in red, and examples that include formulas, structural formulas, ball-and-stick models, and names. Compound names include alkene, alkyne, alcohol, ether, aldehyde, ketone, carboxylic acid, ester, amine, and amide. Alkenes have a double bond. A formula is C subscript 2 H subscript 4 which is named ethene. The ball-and-stick model shows two black balls forming a double bond and each is bonded to two white balls. Alkynes have a triple bond. A formula is C subscript 2 H subscript 2 which is named ethyne. The ball-and-stick model shows two black balls with a triple bond between them each bonded to one white ball. Alcohols have an O H group. The O has two pairs of electron dots. A formula is C H subscript 3 C H subscript 2 O H which is named ethanol. The ball-and-stick model shows two black balls and one red ball bonded to each other with a single bond. There are four white balls visible. Ethers have an O atom in the structure between two R groups. The O atom has two sets of electron dots. A formula is (C subscript 2 H subscript 5) subscript 2 O which is named ethanal. The ball-and-stick model shows two black balls bonded to a red ball which is bonded to two more black balls. All bonds are single. There are five white balls visible. Aldehydes have a C atom to which a double bonded O and an H and an R are included in the structure. The O atom has two sets of electron dots. A formula is C H subscript 3 C H O which is named Ethanal. The ball-and-stick model shows two black bonds bonded to two red balls. The ball-and-stick model shows two black balls bonded with a single bond and the second black ball forms a double bond with a red ball. There are three white balls visible. Ketones show a C atom to which a double bonded O is attached. The left side of the C atom is bonded to R and the right side is bonded to R prime. The O atom as two sets of electron dots. The formula is C H subscript 3 C O C H subscript 2 C H subscript 3 and is named methyl ethyl ketone. The ball-and-stick models shows four black balls all forming single bonds with each other. The second black ball forms a double bond with a red ball. There are five white balls visible. Carboxylic acids have a C to which a double bonded O and an O H are included in the structure. Each O atom has two sets of electron dots. A formula is C H subscript 3 C O O H which is named ethanoic or acetic acid. The ball-and-stick model shows two black balls and one red ball forming single bonds with each other. The second black ball also forms a double bond with another red ball. Three white balls are visible. Esters have a C atom which forms a double bond with an O atom and single bond with another O atom which has an attached hydrocarbon group in the structure. Each O atom has two sets of electron dots. A formula is C H subscript 3 C O subscript 2 C H subscript 2 C H subscript 3 which is named ethyl acetate. The ball-and-stick model shows two black balls, a red ball, and two more black balls forming single bonds with each other. The second black ball forms a double bond with another red ball. There are five white balls visible. Amines have an N atom in the structure to which three hydrocarbon groups, two hydrocarbon groups and one H atom, or one hydrocarbon group and two H atoms may be bonded. Each n has a single set of electron dots. A formula is C subscript 2 H subscript 5 N H subscript 2 which is named ethylamine. The ball-and-stick model shows two black balls and one blue ball forming single bonds with each other. There are five white balls visible. Amides have a C to which a double bonded O and single N incorporated in a structure between two hydrocarbon groups. One hydrocarbon group is bonded to the C, the other to the N. Amides can also have a H atom bonded to the N. The O atom as two sets of electron dots, and the N atom has one set. A formula is C H subscript 3 C O N H subscript 2 which is named ethanamide or acetamide. The ball-and-stick model shows two black balls and one blue ball forming single bonds with each other. The second black ball forms a double bond with one red ball. There are four white balls visible.

Examples

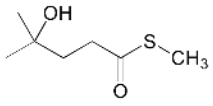
1. Identify the functional groups (other than alkanes) in the following organic compounds. State whether alcohols and amines are primary, secondary, or tertiary.

a)

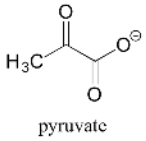


penicillin

b)

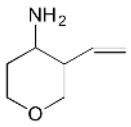


c)



pyruvate

d)



Solutions to exercises

2. Draw one example each of compounds fitting the descriptions below, using line structures. Be sure to designate the location of all non-zero formal charges. All atoms should have complete octets (phosphorus may exceed the octet rule). There are many possible correct answers for these, so be sure to check your structures with your instructor or tutor.

a) a compound with molecular formula $C_6H_{11}NO$ that includes alkene, secondary amine, and primary alcohol functional groups

b) an ion with molecular formula $C_3H_5O_6P^{2-}$ that includes aldehyde, secondary alcohol, and phosphate functional groups.

c) A compound with molecular formula C_6H_9NO that has an amide functional group and does *not* have an alkene group.

10.3: Functional groups is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

10.4: Case Study- The Molecular Tapestry of Healing

Introduction: The intricate world of organic chemistry is not confined to textbooks and laboratories; it unfolds in the development of drugs that treat, heal, and save lives. The sketching of organic structures and the unraveling of organic reactions are crucial in understanding how drugs work. This case study delves into the personal dimension of how pharmacologists apply these concepts to drug mechanisms of action.

Scenario: In the quiet hum of the research wing at Nova Pharmaceuticals, Dr. Nina Patel, with her years of experience as a pharmacologist, stands contemplatively before a vast whiteboard. It's her task, and passion, to bring clarity to the complex interaction between a new cardiovascular drug and the body's chemistry. With a steady hand, she begins to draw. Each line represents bonds; each circle, atoms. Her team gathers, watching as the drug's structure takes shape, transforming from mere lines and curves into a representation of hope for patients in need.

Drawing Organic Structures and Understanding Reactions: As Dr. Patel's marker glides across the board, the drug's molecular structure becomes a focal point for discussion. She points out the functional groups that will engage with cellular receptors and how the drug's form will influence its function. With each stroke, she not only sketches a molecule but also maps out the journey it will take through the body, predicting its metabolic fate.

Case Study Questions:

1. **How can drawing organic structures aid in understanding drug interactions?**
2. **Why is knowledge of organic reactions important in drug development?**

Hands-On Classroom Activities:

1. **Organic Structure Models:** In the "Organic Structure Models" activity, students will employ molecular model kits to construct the organic structures of common drugs, after which they will engage in a discussion about the functions and roles of these drugs based on their molecular configurations.
2. **Reaction Role-Play**: The "Reaction Role-Play" activity involves students taking on the roles of enzymes and substrates to act out chemical reactions, thereby demonstrating how organic reactions are pivotal in drug metabolism and influence the efficacy of pharmaceuticals within the body.

Conclusion: For Dr. Patel, the organic structures, and reactions she elucidates are more than scientific concepts; they are the narratives of molecules that will one day circulate in the bloodstream of patients, battling disease. This case study showcases how the personal dedication of pharmacologists like Dr. Patel to understanding the organic chemistry of drugs can lead to profound impacts on patient health. Their ability to draw and interpret the subtle language of organic molecules is instrumental in transforming raw chemical compounds into life-saving medications.

10.4: Case Study- The Molecular Tapestry of Healing is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

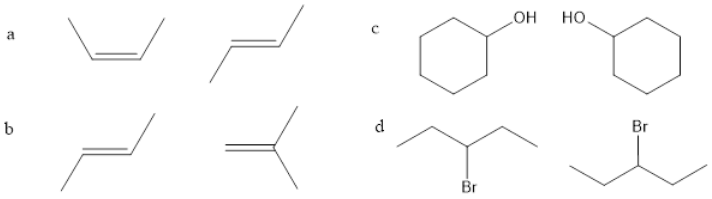
10.5: 3D Printing Activity- Cyclohexane

10.5: 3D Printing Activity- Cyclohexane is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

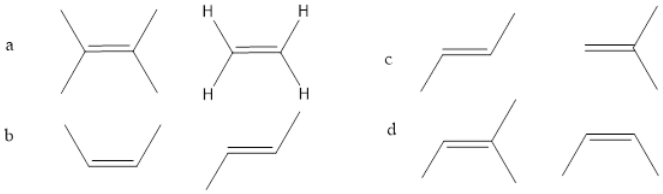
10.E: Exercises

Multiple-Choice Problems

1. Which of the following are structural isomers?



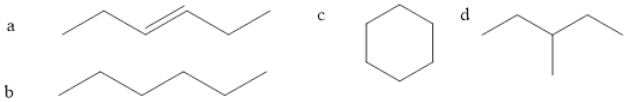
2. Which of the following pairs are cis trans isomers?



3. What is the name for an eight-carbon unbranched alkane chain?

   a. hexane
   b. heptane
   c. octane
   d. nonane
   e. decane

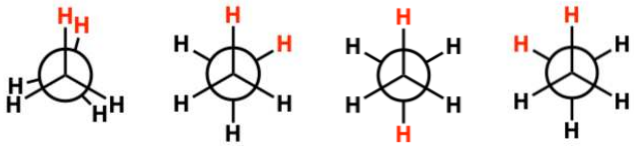
4. Which of the following compounds are saturated hydrocarbons?



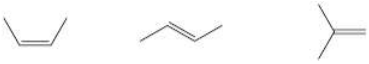
5. Which of the following alkanes has the lowest boiling point?

   a. ethane
   b. propane
   c. butane
   d. pentane

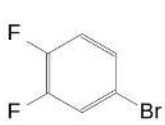
6. Which of the following has the highest energy?



7. Which of the following is a cis isomer:



8. Which of the following is the correct name for the following compound?

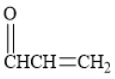
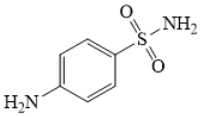
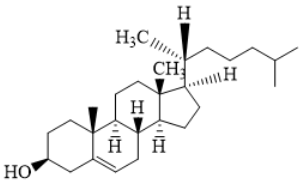
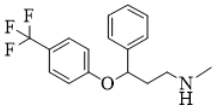


   a. 4-bromo-1,2-difluorobenzene
   b. 1,2-difluoro-3-bromobenzene
   c. 1,1-difluoro-2-bromobenzene

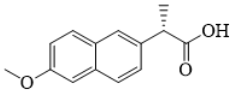
d. 1-bromo-3-fluorobenzene

9. Which of the following statements is false for the compound phenol?
    a. Phenol is a benzene derived compound.
    b. Phenol is highly toxic to the body even in small doses.
    c. Phenol can be used as a catalyst in the hydrogenation of benzene into cyclohexane.
    d. Phenol is used as an antiseptic in minute doses.
10. In a reaction, compound L with the molecular formula C_3H_8O is converted to compound Z with the formula C_3H_6O. L is:
    a. oxidized
    b. reduced
    c. dehydrated
    d. none of these
11. Which of the following would you expect to be soluble in water?
    a. CH_3OCH_3
    b. CH_3CH_2OH
    c. $CH_3CH_2OCH\ {}_2CH_2CH_3$
    d. $CH_3(CH_2)_3OH$

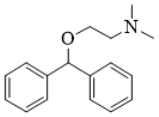
Practice Problems

1. Draw line structures from the following condensed structures.
    a. $CH_3CH_2CH_2OH$
    b. $CH_3CH_2CH_2OCH(CH_3)_2$
    c. 
    d. 
    e. CH_3COCH_2Cl
    f. $CH_3CO_2CH_2CH_3$
    g. $(CH_3CH_2)_3CCH{=}CH_3$
2. Write molecular formulas for the following molecules.
    a. Sulfonilamide, an antibiotic
    
    b. Cholesterol
    
    c. Fluoxetine, an antidepressant
    

d. Naproxen, an anti-inflammatory drug

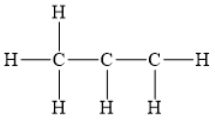


e. Diphenhydramine, an antihistamine

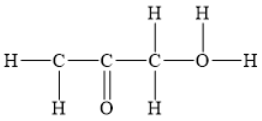


3. Identify the following functional groups in molecules from the previous problem: amine, carboxylic acid, ether, aromatic, alcohol, alkyl halide.
4. Find mistakes in the following Lewis structures, then draw a correct related structure with the same molecular formula. If there are no problems with a given structure, write “correct”.

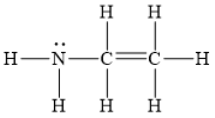
a.



b.

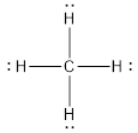


c.

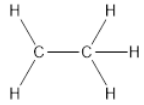


5. Find mistakes in the following Lewis structures, then draw a correct related structure with the same molecular formula. If there are no problems with a given structure, write “correct”.

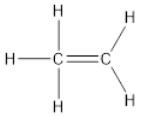
a



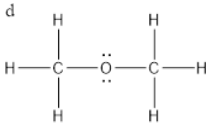
c



b



d



6. Which of the following would you expect to be soluble in water?
   a. Vitamin C
   b. serotonin
   c. caffeine
   d. benzene
7. Name the following acyclic hydrocarbons.
   a. CH_4
   b. CH_3CH_3
   c. $CH_3CH_2CH_3$
   d. $CH_3CH_2CH_2CH_3$
8. Name the following compounds:

a.



b.



c.



d.



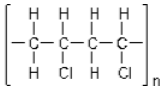
e.



f.



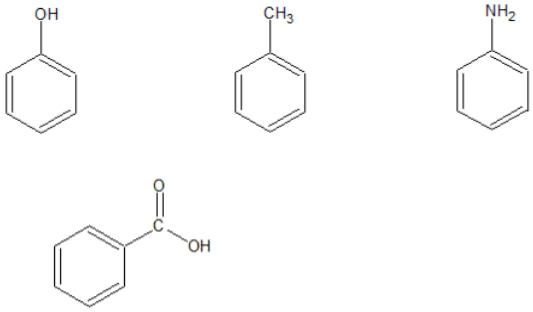
9. Name three properties of hydrocarbons.
10. What are the products of a combustion reaction?
11. What is the monomer of PVC?



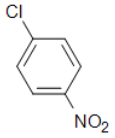
12. Which of the following are aromatic compounds?

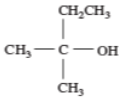
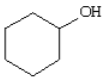
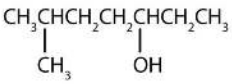


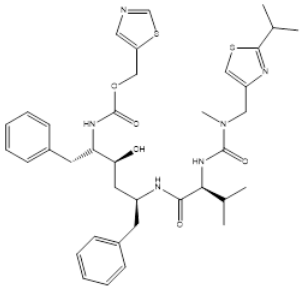
13. Name the following compounds.



14. Name the following compound using OMP nomenclature:



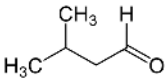
15. What is the functional group of 1-propanol, $CH_3CH_2CH_2OH$?
16. What is the functional group of chlorobutane, $CH_3CH_2CH_2CH_2Cl$?
17. Name each alcohol and classify them as primary, secondary, or tertiary.
    a. $CH_3CH_2CH_2CH_2CH_2OH$
    b. 
    c. 
    d. 
    e. 
18. Draw the structure for each of the following alcohols.
    a. 3-pentanol
    b. 2,2-dimethyl-3-butanol
    c. cyclopropanol
    d. 3-methyl-2-hexanol
    e. 3-ethyl-3,4-dimethyl-2-heptanol
19. Why is methanol more soluble in water than 1-heptanol?
20. Why does 1-propanol have a lower boiling point than 1-heptanol?
21. Arrange these alcohols in order of increasing boiling point: 1-pentanol, methanol, and 1-hexanol.
22. Draw the structure of glycerol, $(HOCH_2)_2CHOH$.
23. Rank the following compounds in order of increasing boiling point:
    a. CH_3OCH_3
    b. $CH_3(CH_2)_2O(CH_2)_2CH_3$
    c. $CH_3(CH_2)_3OH$
    d. CH_3CH_2OH
24. Rank the following compounds in order of increasing boiling point:
    a. CH_3CH_2I
    b. CH_3CH_2Br
    c. CH_3CH_2Cl
25. Rank the following compounds in order of increasing boiling point:
    a. CH_3CH_2I
    b. CH_3CH_3
    c. $CH_3CH_2CH_2I$
26. Circle all the chiral centers in ritonavir.



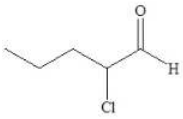
ritonavir

27. Draw the ketone and aldehyde isomers of compounds containing the chemical formula of C_3H_6O.
28. Name the following compounds.

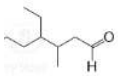
a.



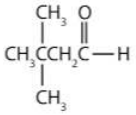
b.



c.



d.

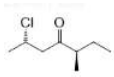


29. Name the following compounds.

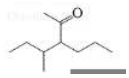
a.



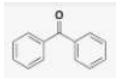
b.



c.



d.



30. Which compound in each pair has the higher boiling point? Why?

a. propanol and propanal
b. propane and 2-propanone
c. 2-propanone and 2-butanone

10.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

11: Organic Chemistry Reactions

11.1: Organic Reactions

11.2: Alcohols and Ethers

11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters

11.4: Amines and Amides

11.E: Exercises

11: Organic Chemistry Reactions is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

11.1: Organic Reactions

35

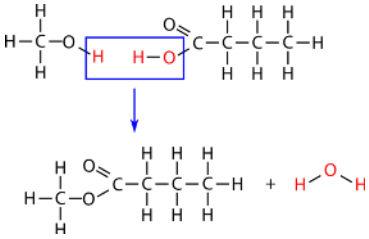
Harper College Chemistry Department

Derived from Foundations of Introductory Chemistry-1 by LibreTexts and Chemistry: Atoms First by OpenStax

Condensation Reactions

A **condensation reaction** is a reaction in which two molecules combine to form a single molecule. A small molecule, often water, is usually removed during a condensation reaction.

An **esterification** is a condensation reaction in which an ester is formed from an alcohol and a carboxylic acid. Esterification is a subcategory of condensation reactions because a water molecule is produced in the reaction. The reaction is catalyzed by a strong acid, usually sulfuric acid. When the carboxylic acid butanoic acid is heated with an excess of methanol and a few drops of sulfuric acid, the ester methyl butanoate is produced. Methyl butanoate has the scent of pineapples. The reaction is shown below with both molecular and structural formulas.



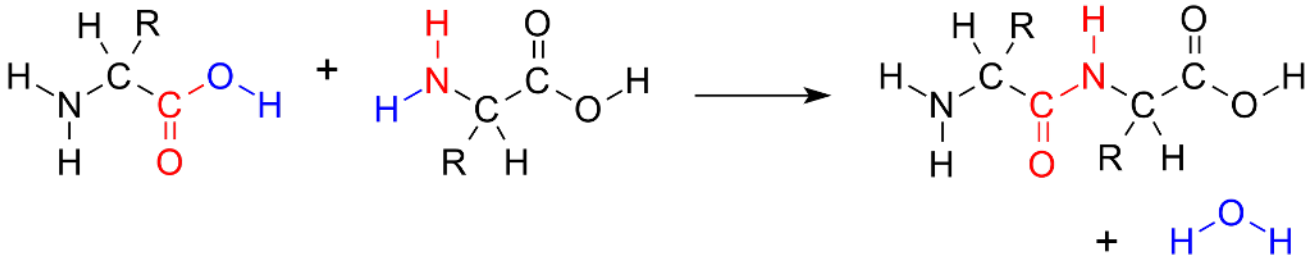
Saponification describes the alkaline hydrolysis reaction of an ester. The term saponification originally described the hydrolysis of long-chain esters called fatty acid esters to produce soap molecules, which are the salts of fatty acids. One such soap molecule is sodium stearate, formed from the hydrolysis of ethyl stearate.

“>$C_{17}H_{35}COOC_2H_5 + NaOH \rightarrow C_{17}H_{35}COO^{-}Na^{+} + C_2H_5OH$
ethyl stearate sodium hydroxide sodium stearate (soap) ethanol

The sodium hydroxide is not acting as a catalyst, but is consumed in the reaction.

Amidation reactions

Amino acids are important biological molecules that have an amine functional group on one end of the molecule and a carboxylic acid functional group on the other end. When two amino acids combine in a condensation reaction, a covalent bond forms between the amine nitrogen of one amino acid and the carboxyl carbon of the second amino acid. A molecule of water is then removed as a secondary product.



Amino acids join together to form a molecule called a dipeptide. The
“>−OH
from the carboxylic acid group of one amino acid combines with a hydrogen atom from the amine group of the other amino acid to produce water (blue).

This reaction forms a molecule called a dipeptide and the carbon-nitrogen covalent bond is called a peptide bond. When repeated numerous times, a lengthy molecule called a protein is eventually produced.

Polymerization – Addition Polymers

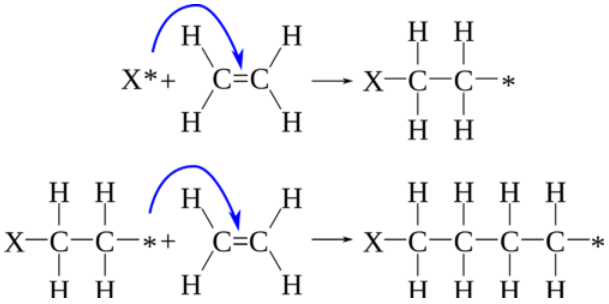
We enjoy the benefits of Styrofoam containers, but don't often think about where they end up. Styrofoam materials do not break down quickly under exposure to the elements. When buried in a landfill, styrofoam will remain intact for a long time. The good news is that there is not a lot of this pollutant found in landfills (maybe about “>0.5% by weight of the total mass of garbage). There is no good way to recycle Styrofoam at present, but someday a creative scientist may come up with one.

Polymers are very different from the other kinds of organic molecules that you have seen so far. Whereas other compounds are of relatively low molar mass, polymers are giant molecules of very high molar mass. Polymers are the primary components of all sorts of plastics and related compounds. A **polymer** is a large molecule formed of many smaller molecules covalently bonded in a repeating pattern. The small molecules which make up the polymer are called **monomers**. Polymers generally form either from an addition reaction or a condensation reaction.

An **addition polymer** is a polymer formed by chain addition reactions between monomers that contain a double bond. Molecules of ethene can polymerize with each other under the right conditions to form the polymer called polyethylene.

“>nCH2=CH2 → −(CH2CH2)n−

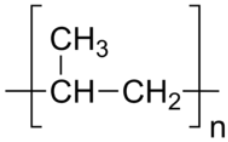
The letter “>n stands for the number of monomers that are joined in repeated fashion to make the polymer and can have a value in the hundreds or even thousands.



Polyethylene synthesis.

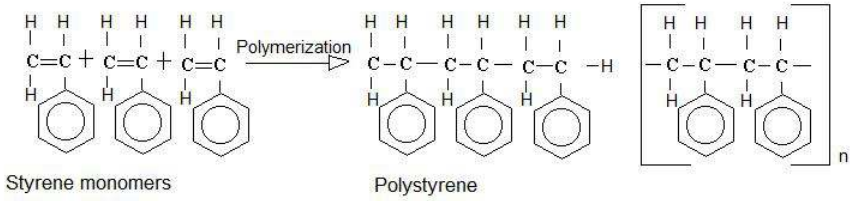
Polyethylene can have different properties depending on the length of the polymer chains and on how efficiently they pack together. Some common products made from different forms of polyethylene include plastic bottles, plastic bags, and harder plastic objects such as milk crates.

Several other kinds of unsaturated monomers can be polymerized and are components in common household products. Polypropylene is stiffer than polyethylene and is in plastic utensils and some other types of containers.



Polypropylene structure.

Polystyrene is used in insulation and in molded items such as coffee cups.



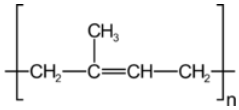
Polystyrene synthesis and structure.

Polyvinyl chloride (PVC) is extensively used for plumbing pipes.



Polyvinyl chloride.

Polyisoprene is a polymer of isoprene and is better known as rubber. It is produced naturally by rubber trees, but several variants have been developed which demonstrate improvements on the properties of natural rubber.



For your information: KEVLAR

Kevlar (Figure 2) is a synthetic polymer made from two monomers 1,4-phenylene-diamine and terephthaloyl chloride (Kevlar is a registered trademark of DuPont). Kevlar's first commercial use was as a replacement for steel in racing tires. Kevlar is typically spun into ropes or fibers. The material has a high tensile strength-to-weight ratio (it is about 5 times stronger than an equal weight of steel), making it useful for many applications from bicycle tires to sails to body armor.

A structural formula is shown for the polymer Kevlar. The structure appears inside brackets which have single dashes extending from them at the left and right ends. Outside the lower right corner of the brackets, an italicized n appears. The structure inside the brackets includes a C atom forming a double bond with an O atom and a bond with a benzene ring. The benzene ring forms a bond with another C atom which has a double bond with an O atom. The C atom is bonded to an N atom. The N atom is bonded to an H atom and a benzene ring. The benzene ring bonds with another N atom which is also bonded to an H atom.

This illustration shows the formula for polymeric Kevlar.

The material owes much of its strength to hydrogen bonds between polymer chains (refer back to the chapter on intermolecular interactions). These bonds form between the carbonyl group oxygen atom (which has a partial negative charge due to oxygen's electronegativity) on one monomer and the partially positively charged hydrogen atom in the N–H bond of an adjacent monomer in the polymer structure (see dashed line in Figure 3). There is additional strength derived from the interaction between the unhybridized *p* orbitals in the six-membered rings, called aromatic stacking.

This diagram shows the repeating, interlinked units that exist in Kevlar, taking on a sheet-like appearance. Dashed line segments are indicated between units. Individual units are composed of nitrogen, hydrogen, oxygen and carbon atoms. The repeating structural units include benzene rings and double bonds.

The diagram shows the polymer structure of Kevlar, with hydrogen bonds between polymer chains represented by dotted lines.

Kevlar may be best known as a component of body armor, combat helmets, and face masks. Since the 1980s, the US military has used Kevlar as a component of the PASGT (personal armor system for ground troops) helmet and vest. Kevlar is also used to protect armored fighting vehicles and aircraft carriers. Civilian applications include protective gear for emergency service personnel such as body armor for police officers and heat-resistant clothing for fire fighters. Kevlar based clothing is considerably lighter and thinner than equivalent gear made from other materials (Figure 4).

Three photos are shown. In the first, two male soldiers are shown sorting through green brown material on a table. In the second, two people are shown paddling a canoe. In the third, heavy white rope is being manipulated with a hand tool.

(a) These soldiers are sorting through pieces of a Kevlar helmet that helped absorb a grenade blast. Kevlar is also used to make (b) canoes and (c) marine mooring lines. (credit a: modification of work by "Cla68"/Wikimedia Commons; credit b: modification of work by "OakleyOriginals"/Flickr; credit c: modification of work by Casey H. Kyhl)

In addition to its better-known uses, Kevlar is also often used in cryogenics for its very low thermal conductivity (along with its high strength). Kevlar maintains its high strength when cooled to the temperature of liquid nitrogen (–196 °C).

11.1: Organic Reactions is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

11.2: Alcohols and Ethers

Learning Objectives

By the end of this section, you will be able to:

- Describe the structure and properties of alcohols
- Describe the structure and properties of ethers
- Name and draw structures for alcohols and ethers

In this section, we will learn about alcohols and ethers.

11.2.1: Alcohols

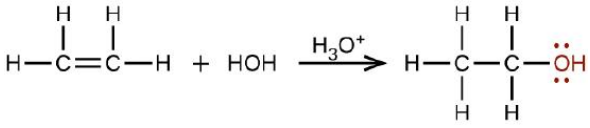
Incorporation of an oxygen atom into carbon- and hydrogen-containing molecules leads to new functional groups and new families of compounds. When the oxygen atom is attached by single bonds, the molecule is either an alcohol or ether.

Alcohols are derivatives of hydrocarbons in which an –OH group has replaced a hydrogen atom. Although all alcohols have one or more hydroxyl (–OH) functional groups, they do not behave like bases such as NaOH and KOH. NaOH and KOH are ionic compounds that contain OH^- ions. Alcohols are covalent molecules; the –OH group in an alcohol molecule is attached to a carbon atom by a covalent bond.

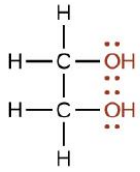
Ethanol, CH_3CH_2OH, also called ethyl alcohol, is a particularly important alcohol for human use. Ethanol is the alcohol produced by some species of yeast that is found in wine, beer, and distilled drinks. It has long been prepared by humans harnessing the metabolic efforts of yeasts in fermenting various sugars:

$$\underset{\text{glucose}}{C_6H_{12}O_6(aq)} \xrightarrow{\text{Yeast}} \underset{\text{ethanol}}{2C_2H_5OH(aq)} + 2CO_2(g)$$

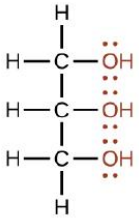
Large quantities of ethanol are synthesized from the addition reaction of water with ethylene using an acid as a catalyst:



Alcohols containing two or more hydroxyl groups can be made. Examples include 1,2-ethanediol (ethylene glycol, used in antifreeze) and 1,2,3-propanetriol (glycerine, used as a solvent for cosmetics and medicines):



1,2-ethanediol



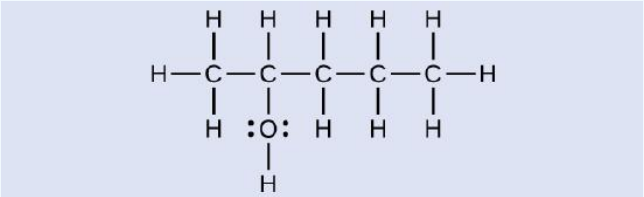
1,2,3-propanetriol

11.2.1.1: Naming Alcohols

The name of an alcohol comes from the hydrocarbon from which it was derived. The final *-e* in the name of the hydrocarbon is replaced by *-ol*, and the carbon atom to which the –OH group is bonded is indicated by a number placed before the name.[5]

Example 11.2.1: Naming Alcohols

Consider the following example. How should it be named?

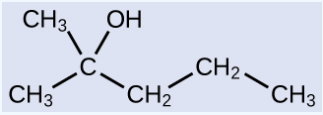


Solution

The carbon chain contains five carbon atoms. If the hydroxyl group was not present, we would have named this molecule pentane. To address the fact that the hydroxyl group is present, we change the ending of the name to *-ol*. In this case, since the –OH is attached to carbon 2 in the chain, we would name this molecule 2-pentanol.

Exercise 11.2.1

Name the following molecule:

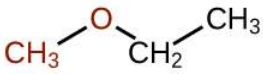


Answer

2-methyl-2-pentanol

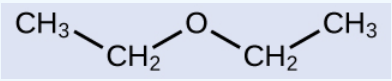
11.2.2: Ethers

Ethers are compounds that contain the functional group –O–. Ethers do not have a designated suffix like the other types of molecules we have named so far. In the IUPAC system, the oxygen atom and the smaller carbon branch are named as an alkoxy substituent and the remainder of the molecule as the base chain, as in alkanes. As shown in the following compound, the red symbols represent the smaller alkyl group and the oxygen atom, which would be named “methoxy.” The larger carbon branch would be ethane, making the molecule methoxyethane. Many ethers are referred to with common names instead of the IUPAC system names. For common names, the two branches connected to the oxygen atom are named separately and followed by “ether.” The common name for the compound shown in Example **11.2.2** is ethylmethyl ether:



Example 11.2.2: Naming Ethers

Provide the IUPAC and common name for the ether shown here:



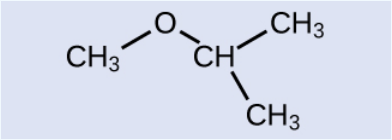
Solution

IUPAC: The molecule is made up of an ethoxy group attached to an ethane chain, so the IUPAC name would be ethoxyethane.

Common: The groups attached to the oxygen atom are both ethyl groups, so the common name would be diethyl ether.

Exercise 11.2.1

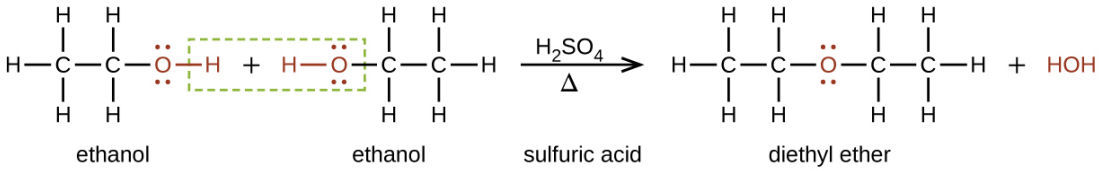
Provide the IUPAC and common name for the ether shown:



Answer

IUPAC: 2-methoxypropane; common: isopropylmethyl ether

Ethers can be obtained from alcohols by the elimination of a molecule of water from two molecules of the alcohol. For example, when ethanol is treated with a limited amount of sulfuric acid and heated to 140 °C, diethyl ether and water are formed:



In the general formula for ethers, R—**O**—R, the hydrocarbon groups (R) may be the same or different. Diethyl ether, the most widely used compound of this class, is a colorless, volatile liquid that is highly flammable. It was first used in 1846 as an anesthetic, but better anesthetics have now largely taken its place. Diethyl ether and other ethers are presently used primarily as solvents for gums, fats, waxes, and resins. *Tertiary*-butyl methyl ether, $C_4H_9OCH_3$ (abbreviated MTBE—italicized portions of names are not counted when ranking the groups alphabetically—so butyl comes before methyl in the common name), is used as an additive for gasoline. MTBE belongs to a group of chemicals known as oxygenates due to their capacity to increase the oxygen content of gasoline.

Link to Learning

Want more practice naming ethers? This brief video review summarizes the nomenclature for ethers.

Chemistry in Everyday Life: Carbohydrates and Diabetes

Carbohydrates are large biomolecules made up of carbon, hydrogen, and oxygen. The dietary forms of carbohydrates are foods rich in these types of molecules, like pastas, bread, and candy. The name “carbohydrate” comes from the formula of the molecules, which can be described by the general formula $C_m(H_2O)_n$, which shows that they are in a sense “carbon and water” or “hydrates of carbon.” In many cases, *m* and *n* have the same value, but they can be different. The smaller carbohydrates are generally referred to as “sugars,” the biochemical term for this group of molecules is “saccharide” from the Greek word for sugar (Figure 20.12). Depending on the number of sugar units joined together, they may be classified as monosaccharides (one sugar unit), disaccharides (two sugar units), oligosaccharides (a few sugars), or polysaccharides (the polymeric version of sugars—polymers were described in the feature box earlier in this chapter on recycling plastics). The scientific names of sugars can be recognized by the suffix *-ose* at the end of the name (for instance, fruit sugar is a monosaccharide called “fructose” and milk sugar is a disaccharide called lactose composed of two monosaccharides, glucose and galactose, connected together). Sugars contain some of the functional groups we have discussed: Note the alcohol groups present in the structures and how monosaccharide units are linked to form a disaccharide by formation of an ether.

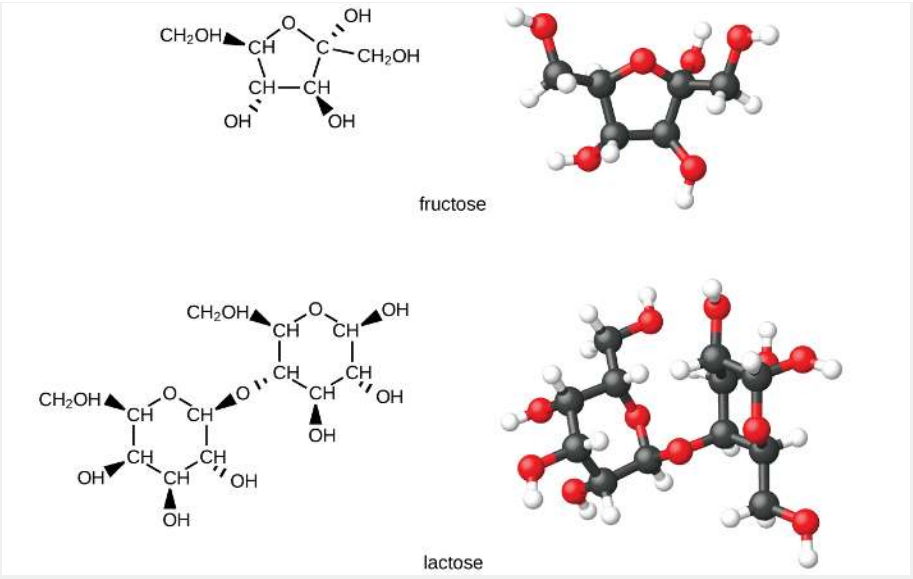


Figure 20.12 The illustrations show the molecular structures of fructose, a five-carbon monosaccharide, and of lactose, a disaccharide composed of two isomeric, six-carbon sugars.

Organisms use carbohydrates for a variety of functions. Carbohydrates can store energy, such as the polysaccharides glycogen in animals or starch in plants. They also provide structural support, such as the polysaccharide cellulose in plants and the modified polysaccharide chitin in fungi and animals. The sugars ribose and deoxyribose are components of the backbones of RNA and DNA, respectively. Other sugars play key roles in the function of the immune system, in cell-cell recognition, and in many other biological roles.

Diabetes is a group of metabolic diseases in which a person has a high sugar concentration in their blood (Figure **11.2.1**). Diabetes may be caused by insufficient insulin production by the pancreas or by the body's cells not responding properly to the insulin that is produced. In a healthy person, insulin is produced when it is needed and functions to transport glucose from the blood into the cells where it can be used for energy. The long-term complications of diabetes can include loss of eyesight, heart disease, and kidney failure.

In 2013, it was estimated that approximately 3.3% of the world's population (~380 million people) suffered from diabetes, resulting in over a million deaths annually. Prevention involves eating a healthy diet, getting plenty of exercise, and maintaining a normal body weight. Treatment involves all of these lifestyle practices and may require injections of insulin.

Even after treatment protocols were introduced, the need to continually monitor their glucose levels posed a challenge for people with diabetes. The first tests required a doctor or lab, and therefore limited access and frequency. Eventually, researchers developed small tablets that would react to the presence of glucose in urine, but these still required a relatively complex process. Chemist Helen Free, who was working on improvements to the tablets, conceived a simpler device: a small test strip. With her husband and research partner, Alfred Free, she produced the first such product for measuring glucose; soon after, she expanded the technology to provide test strips for other compounds and conditions. While very recent advances (such as breath tests, discussed earlier in the text) have shown promise in replacing test strips, they have been widely used for decades and remain a primary method today.



Figure **11.2.1**: Diabetes is a disease characterized by high concentrations of glucose in the blood. Treating diabetes involves making lifestyle changes, monitoring blood-sugar levels, and sometimes insulin injections. (credit: "Blausen Medical Communications"/Wikimedia Commons)

11.2.3: Footnotes

- 5The IUPAC adopted new nomenclature guidelines in 2013 that require this number to be placed as an "infix" rather than a prefix. For example, the new name for 2-propanol would be propan-2-ol. Widespread adoption of this new nomenclature will take some time, and students are encouraged to be familiar with both the old and new naming protocols.

This page titled 11.2: Alcohols and Ethers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **20.2: Alcohols and Ethers** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters

Learning Objectives

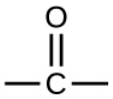
By the end of this section, you will be able to:

- Describe the structure and properties of aldehydes, ketones, carboxylic acids and esters

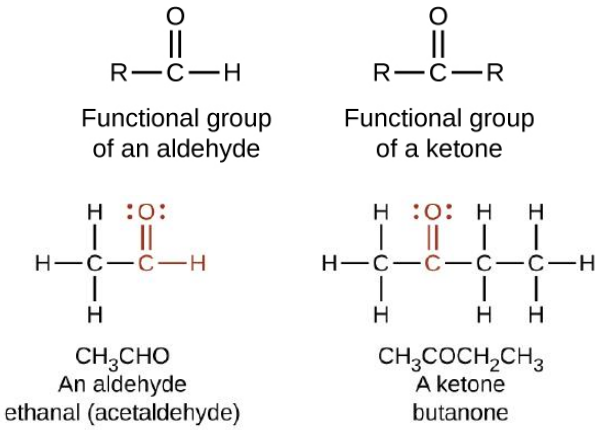
Another class of organic molecules contains a carbon atom connected to an oxygen atom by a double bond, commonly called a carbonyl group. The trigonal planar carbon in the carbonyl group can attach to two other substituents leading to several subfamilies (aldehydes, ketones, carboxylic acids and esters) described in this section.

11.3.1: Aldehydes and Ketones

Both aldehydes and ketones contain a carbonyl group, a functional group with a carbon-oxygen double bond. The names for aldehyde and ketone compounds are derived using similar nomenclature rules as for alkanes and alcohols, and include the class-identifying suffixes *-al* and *-one*, respectively:



In an aldehyde, the carbonyl group is bonded to at least one hydrogen atom. In a ketone, the carbonyl group is bonded to two carbon atoms:



As text, an aldehyde group is represented as –CHO; a ketone is represented as –C(O)– or –CO–.

In both aldehydes and ketones, the geometry around the carbon atom in the carbonyl group is trigonal planar; the carbon atom exhibits sp^2 hybridization. Two of the sp^2 orbitals on the carbon atom in the carbonyl group are used to form σ bonds to the other carbon or hydrogen atoms in a molecule. The remaining sp^2 hybrid orbital forms a σ bond to the oxygen atom. The unhybridized *p* orbital on the carbon atom in the carbonyl group overlaps a *p* orbital on the oxygen atom to form the π bond in the double bond.

Like the

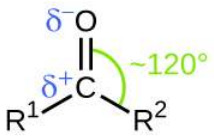
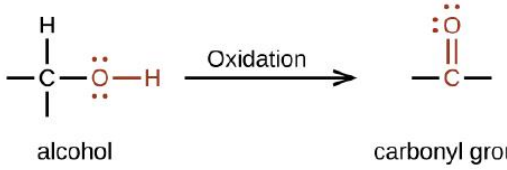


Figure **11.3.1**: The carbonyl group is polar, and the geometry of the bonds around the central carbon is trigonal planar.

The importance of molecular structure in the reactivity of organic compounds is illustrated by the reactions that produce aldehydes and ketones. We can prepare a carbonyl group by oxidation of an alcohol—for organic molecules, oxidation of a carbon atom is said to occur when a carbon-hydrogen bond is replaced by a carbon-oxygen bond. The reverse reaction—replacing a carbon-

oxygen bond by a carbon-hydrogen bond—is a reduction of that carbon atom. Recall that oxygen is generally assigned a –2 oxidation number unless it is elemental or attached to a fluorine. Hydrogen is generally assigned an oxidation number of +1 unless it is attached to a metal. Since carbon does not have a specific rule, its oxidation number is determined algebraically by factoring the atoms it is attached to and the overall charge of the molecule or ion. In general, a carbon atom attached to an oxygen atom will have a more positive oxidation number and a carbon atom attached to a hydrogen atom will have a more negative oxidation number. This should fit nicely with your understanding of the polarity of C–O and C–H bonds. The other reagents and possible products of these reactions are beyond the scope of this chapter, so we will focus only on the changes to the carbon atoms:



Example 11.3.1: Oxidation and Reduction in Organic Chemistry

Methane represents the completely reduced form of an organic molecule that contains one carbon atom. Sequentially replacing each of the carbon-hydrogen bonds with a carbon-oxygen bond would lead to an alcohol, then an aldehyde, then a carboxylic acid (discussed later), and, finally, carbon dioxide:

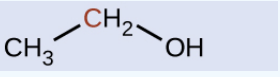
What are the oxidation numbers for the carbon atoms in the molecules shown here?

Solution

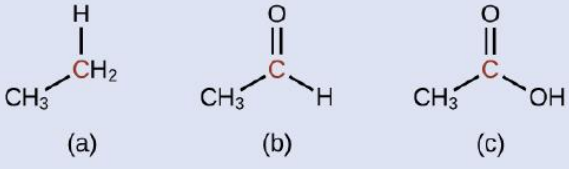
In this example, we can calculate the oxidation number (review the chapter on oxidation-reduction reactions if necessary) for the carbon atom in each case (note how this would become difficult for larger molecules with additional carbon atoms and hydrogen atoms, which is why organic chemists use the definition dealing with replacing C–H bonds with C–O bonds described). For CH_4, the carbon atom carries a –4 oxidation number (the hydrogen atoms are assigned oxidation numbers of +1 and the carbon atom balances that by having an oxidation number of –4). For the alcohol (in this case, methanol), the carbon atom has an oxidation number of –2 (the oxygen atom is assigned –2, the four hydrogen atoms each are assigned +1, and the carbon atom balances the sum by having an oxidation number of –2; note that compared to the carbon atom in CH_4, this carbon atom has lost two electrons so it was oxidized); for the aldehyde, the carbon atom's oxidation number is 0 (–2 for the oxygen atom and +1 for each hydrogen atom already balances to 0, so the oxidation number for the carbon atom is 0); for the carboxylic acid, the carbon atom's oxidation number is +2 (two oxygen atoms each at –2 and two hydrogen atoms at +1); and for carbon dioxide, the carbon atom's oxidation number is +4 (here, the carbon atom needs to balance the –4 sum from the two oxygen atoms).

Exercise 11.3.1

Indicate whether the marked carbon atoms in the three molecules here are oxidized or reduced relative to the marked carbon atom in ethanol:



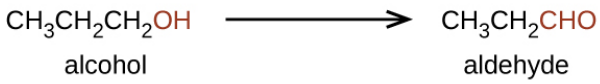
There is no need to calculate oxidation states in this case; instead, just compare the types of atoms bonded to the marked carbon atoms:



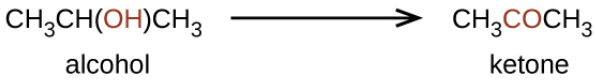
Answer

(a) reduced (bond to oxygen atom replaced by bond to hydrogen atom); (b) oxidized (one bond to hydrogen atom replaced by one bond to oxygen atom); (c) oxidized (2 bonds to hydrogen atoms have been replaced by bonds to an oxygen atom)

Aldehydes are commonly prepared by the oxidation of alcohols whose –OH functional group is located on the carbon atom at the end of the chain of carbon atoms in the alcohol:



Alcohols that have their –OH groups in the middle of the chain are necessary to synthesize a ketone, which requires the carbonyl group to be bonded to two other carbon atoms:



An alcohol with its –OH group bonded to a carbon atom that is bonded to no or one other carbon atom will form an aldehyde. An alcohol with its –OH group attached to two other carbon atoms will form a ketone. If three carbons are attached to the carbon bonded to the –OH, the molecule will not have a C–H bond to be replaced, so it will not be susceptible to oxidation.

Formaldehyde, an aldehyde with the formula HCHO, is a colorless gas with a pungent and irritating odor. It is sold in an aqueous solution called formalin, which contains about 37% formaldehyde by weight. Formaldehyde causes coagulation of proteins, so it kills bacteria (and any other living organism) and stops many of the biological processes that cause tissue to decay. Thus, formaldehyde is used for preserving tissue specimens and embalming bodies. It is also used to sterilize soil or other materials. Formaldehyde is used in the manufacture of Bakelite, a hard plastic having high chemical and electrical resistance.

Dimethyl ketone, CH_3COCH_3, commonly called acetone, is the simplest ketone. It is made commercially by fermenting corn or molasses, or by oxidation of 2-propanol. Acetone is a colorless liquid. Among its many uses are as a solvent for lacquer (including fingernail polish), cellulose acetate, cellulose nitrate, acetylene, plastics, and varnishes; as a paint and varnish remover; and as a solvent in the manufacture of pharmaceuticals and chemicals.

11.3.2: Carboxylic Acids and Esters

The odor of vinegar is caused by the presence of acetic acid, a carboxylic acid, in the vinegar. The odor of ripe bananas and many other fruits is due to the presence of esters, compounds that can be prepared by the reaction of a carboxylic acid with an alcohol. Because esters do not have hydrogen bonds between molecules, they have lower vapor pressures than the alcohols and carboxylic acids from which they are derived (see Figure **11.3.2**).

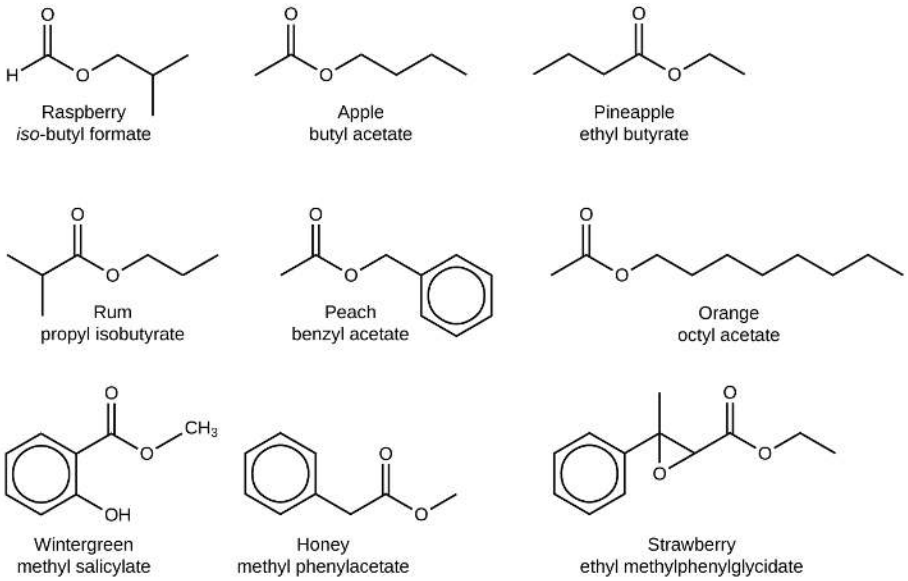
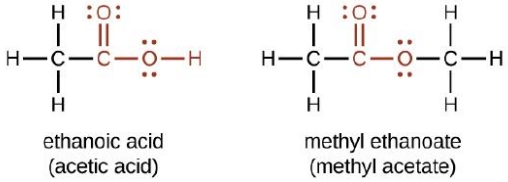


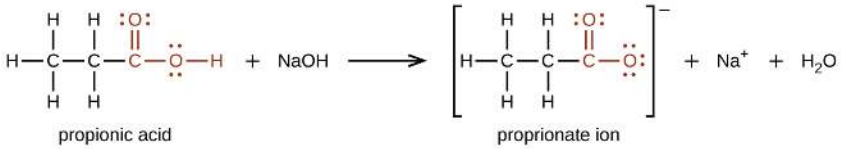
Figure **11.3.2**: Esters are responsible for the odors associated with various plants and their fruits.

Both carboxylic acids and esters contain a carbonyl group with a second oxygen atom bonded to the carbon atom in the carbonyl group by a single bond. In a carboxylic acid, the second oxygen atom also bonds to a hydrogen atom. In an ester, the second oxygen atom bonds to another carbon atom. The names for carboxylic acids and esters include prefixes that denote the lengths of the carbon chains in the molecules and are derived following nomenclature rules similar to those for inorganic acids and salts (see these examples):



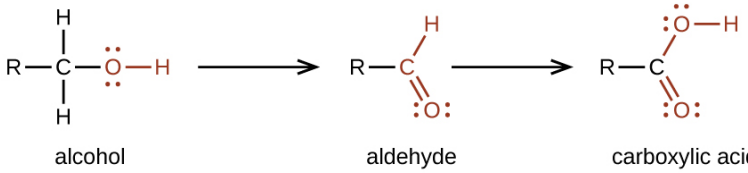
The functional groups for an acid and for an ester are shown in red in these formulas.

The hydrogen atom in the functional group of a carboxylic acid will react with a base to form an ionic salt:

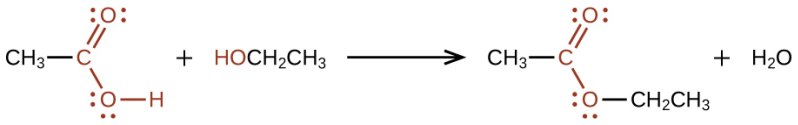


Carboxylic acids are weak acids (see the chapter on acids and bases), meaning they are not 100% ionized in water. Generally only about 1% of the molecules of a carboxylic acid dissolved in water are ionized at any given time. The remaining molecules are undissociated in solution.

We prepare carboxylic acids by the oxidation of aldehydes or alcohols whose –OH functional group is located on the carbon atom at the end of the chain of carbon atoms in the alcohol:



Esters are produced by the reaction of acids with alcohols. For example, the ester ethyl acetate, $CH_3CO_2CH_2CH_3$, is formed when acetic acid reacts with ethanol:



acetic acid ethanol ethyl acetate

The simplest carboxylic acid is formic acid, HCO_2H, known since 1670. Its name comes from the Latin word *formicus*, which means “ant”; it was first isolated by the distillation of red ants. It is partially responsible for the pain and irritation of ant and wasp stings, and is responsible for a characteristic odor of ants that can be sometimes detected in their nests.

Acetic acid, CH_3CO_2H, constitutes 3–6% vinegar. Cider vinegar is produced by allowing apple juice to ferment without oxygen present. Yeast cells present in the juice carry out the fermentation reactions. The fermentation reactions change the sugar present in the juice to ethanol, then to acetic acid. Pure acetic acid has a penetrating odor and produces painful burns. It is an excellent solvent for many organic and some inorganic compounds, and it is essential in the production of cellulose acetate, a component of many synthetic fibers such as rayon.

The distinctive and attractive odors and flavors of many flowers, perfumes, and ripe fruits are due to the presence of one or more esters (Figure **11.3.3**). Among the most important of the natural esters are fats (such as lard, tallow, and butter) and oils (such as linseed, cottonseed, and olive oils), which are esters of the trihydroxyl alcohol glycerine, $C_3H_5(OH)_3$, with large carboxylic acids, such as palmitic acid, $CH_3(CH_2)_{14}CO_2H$, stearic acid, $CH_3(CH_2)_{16}CO_2H$, and oleic acid, Oleic acid is an unsaturated acid; it contains a double bond. Palmitic and stearic acids are saturated acids that contain no double or triple bonds.



Figure **11.3.3**: Over 350 different volatile molecules (many members of the ester family) have been identified in strawberries. (credit: Rebecca Siegel)

This page titled 11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **20.3: Aldehydes, Ketones, Carboxylic Acids, and Esters** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

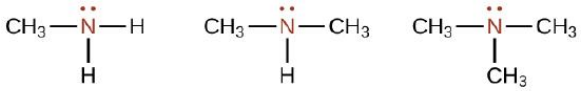
11.4: Amines and Amides

Learning Objectives

By the end of this section, you will be able to:

- Describe the structure and properties of an amine
- Describe the structure and properties of an amide

Amines are molecules that contain carbon-nitrogen bonds. The nitrogen atom in an amine has a lone pair of electrons and three bonds to other atoms, either carbon or hydrogen. Various nomenclatures are used to derive names for amines, but all involve the class-identifying suffix *–ine* as illustrated here for a few simple examples:



methyl amine dimethyl amine trimethyl amine

In some amines, the nitrogen atom replaces a carbon atom in an aromatic hydrocarbon. Pyridine (Figure **11.4.1**) is one such heterocyclic amine. A heterocyclic compound contains atoms of two or more different elements in its ring structure.

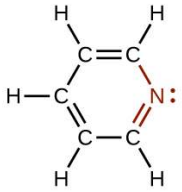


Figure **11.4.1**: The illustration shows one of the resonance structures of pyridine.

How Sciences Interconnect: DNA in Forensics and Paternity

The genetic material for all living things is a polymer of four different molecules, which are themselves a combination of three subunits. The genetic information, the code for developing an organism, is contained in the specific sequence of the four molecules, similar to the way the letters of the alphabet can be sequenced to form words that convey information. The information in a DNA sequence is used to form two other types of polymers, one of which are proteins. The proteins interact to form a specific type of organism with individual characteristics.

A genetic molecule is called DNA, which stands for deoxyribonucleic acid. The four molecules that make up DNA are called nucleotides. Each nucleotide consists of a single- or double-ringed molecule containing nitrogen, carbon, oxygen, and hydrogen called a nitrogenous base. Each base is bonded to a five-carbon sugar called deoxyribose. The sugar is in turn bonded to a phosphate group PO43−)Figure **11.4.2**).

It probably makes sense that the sequence of nucleotides in the DNA of a cat differs from those of a dog. But it is also true that the sequences of the DNA in the cells of two individual pugs differ. Likewise, the sequences of DNA in you and a sibling differ (unless your sibling is an identical twin), as do those between you and an unrelated individual. However, the DNA sequences of two related individuals are more similar than the sequences of two unrelated individuals, and these similarities in sequence can be observed in various ways. This is the principle behind DNA fingerprinting, which is a method used to determine whether two DNA samples came from related (or the same) individuals or unrelated individuals.

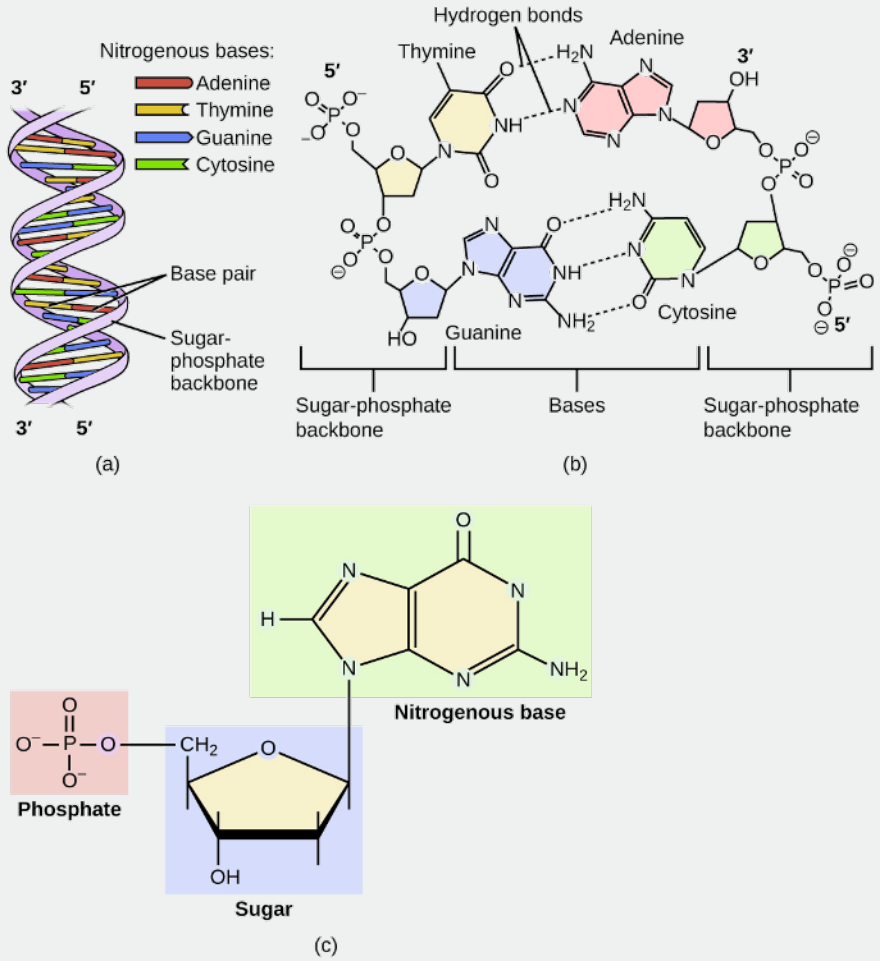


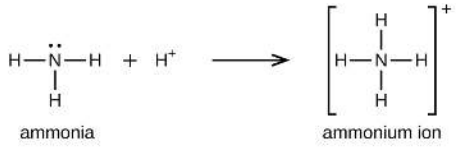
Figure **11.4.2**: DNA is an organic molecule and the genetic material for all living organisms. (a) DNA is a double helix consisting of two single DNA strands hydrogen bonded together at each nitrogenous base. (b) This detail shows the hydrogen bonding (dotted lines) between nitrogenous bases on each DNA strand and the way in which each nucleotide is joined to the next, forming a backbone of sugars and phosphate groups along each strand. (c) This detail shows the structure of one of the four nucleotides that makes up the DNA polymer. Each nucleotide consists of a nitrogenous base (a double-ring molecule, in this case), a five-carbon sugar (deoxyribose), and a phosphate group.

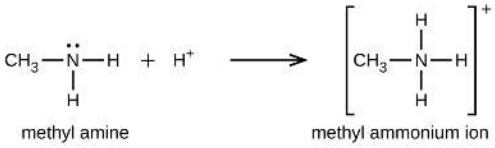
Using similarities in sequences, technicians can determine whether a man is the father of a child (the identity of the mother is rarely in doubt, except in the case of an adopted child and a potential birth mother). Likewise, forensic geneticists can determine whether a crime scene sample of human tissue, such as blood or skin cells, contains DNA that matches exactly the DNA of a suspect.

Link to Learning

Watch this video animation of how DNA is packaged for a visual lesson in its structure.

Like ammonia, amines are weak bases due to the lone pair of electrons on their nitrogen atoms:





The basicity of an amine's nitrogen atom plays an important role in much of the compound's chemistry. Amine functional groups are found in a wide variety of compounds, including natural and synthetic dyes, polymers, vitamins, and medications such as penicillin and codeine. They are also found in many molecules essential to life, such as amino acids, hormones, neurotransmitters, and DNA.

How Sciences Interconnect: Addictive Alkaloids

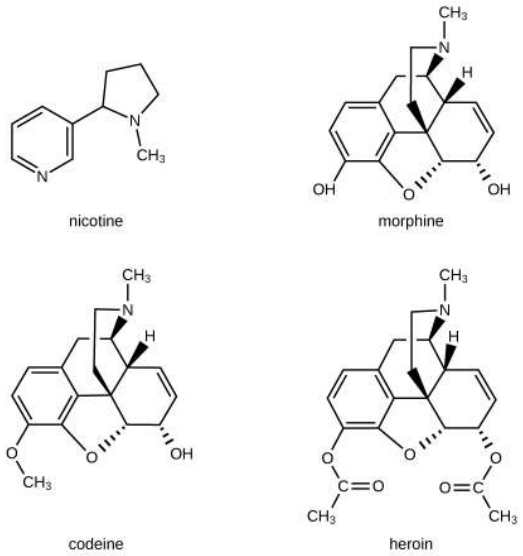
Since ancient times, plants have been used for medicinal purposes. One class of substances, called *alkaloids*, found in many of these plants has been isolated and found to contain cyclic molecules with an amine functional group. These amines are bases. They can react with H_3O^+ in a dilute acid to form an ammonium salt, and this property is used to extract them from the plant:

R3N+H3O++Cl−⟶[R3NH+]Cl−+H2OR3N+H3O++Cl−⟶[R3NH+]Cl−+H2O

The name alkaloid means "like an alkali." Thus, an alkaloid reacts with acid. The free compound can be recovered after extraction by reaction with a base:

R3NH+]Cl−+OH−⟶R3N+H2O+Cl−[R3NH+]Cl−+OH−⟶R3N+H2O+Cl−

The structures of many naturally occurring alkaloids have profound physiological and psychotropic effects in humans. Examples of these drugs include nicotine, morphine, codeine, and heroin. The plant produces these substances, collectively called secondary plant compounds, as chemical defenses against the numerous pests that attempt to feed on the plant:



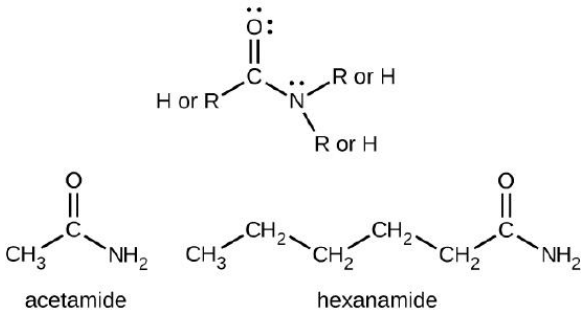
In these diagrams, as is common in representing structures of large organic compounds, carbon atoms in the rings and the hydrogen atoms bonded to them have been omitted for clarity. The solid wedges indicate bonds that extend out of the page. The dashed wedges indicate bonds that extend into the page. Notice that small changes to a part of the molecule change the properties of morphine, codeine, and heroin. Morphine, a strong narcotic used to relieve pain, contains two hydroxyl functional groups, located at the bottom of the molecule in this structural formula. Changing one of these hydroxyl groups to a methyl ether group forms

codeine, a less potent drug used as a local anesthetic. If both hydroxyl groups are converted to esters of acetic acid, the powerfully addictive drug heroin results (Figure **11.4.3**).

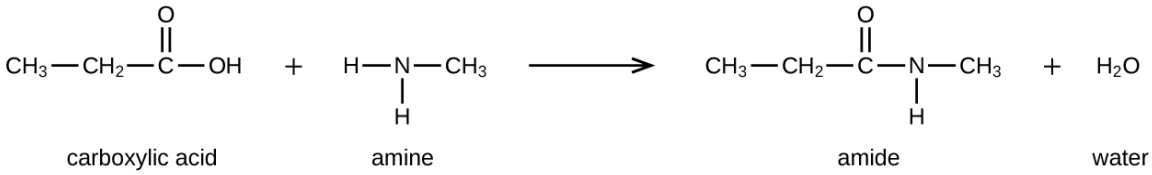


Figure **11.4.3**: Poppies can be used in the production of opium, a plant latex that contains morphine from which other opiates, such as heroin, can be synthesized. (credit: Karen Roe)

Amides are molecules that contain nitrogen atoms connected to the carbon atom of a carbonyl group. Like amines, various nomenclature rules may be used to name amides, but all include use of the class-specific suffix *-amide*:



Amides can be produced when carboxylic acids react with amines or ammonia in a process called amidation. A water molecule is eliminated from the reaction, and the amide is formed from the remaining pieces of the carboxylic acid and the amine (note the similarity to formation of an ester from a carboxylic acid and an alcohol discussed in the previous section):



The reaction between amines and carboxylic acids to form amides is biologically important. It is through this reaction that amino acids (molecules containing both amine and carboxylic acid substituents) link together in a polymer to form proteins.

How Sciences Interconnect: Proteins and Enzymes

Proteins are large biological molecules made up of long chains of smaller molecules called amino acids. Organisms rely on proteins for a variety of functions—proteins transport molecules across cell membranes, replicate DNA, and catalyze metabolic reactions, to name only a few of their functions. The properties of proteins are functions of the combination of amino acids that compose them and can vary greatly. Interactions between amino acid sequences in the chains of proteins result in the folding of the chain into specific, three-dimensional structures that determine the protein's activity.

Amino acids are organic molecules that contain an amine functional group ($–NH_2$), a carboxylic acid functional group (–COOH), and a side chain (that is specific to each individual amino acid). Most living things build proteins from the same 20 different amino acids. Amino acids connect by the formation of a peptide bond, which is a covalent bond formed between two amino acids when the carboxylic acid group of one amino acid reacts with the amine group of the other amino acid. The

formation of the bond results in the production of a molecule of water (in general, reactions that result in the production of water when two other molecules combine are referred to as condensation reactions). The resulting bond—between the carbonyl group carbon atom and the amine nitrogen atom is called a peptide link or peptide bond. Since each of the original amino acids has an unreacted group (one has an unreacted amine and the other an unreacted carboxylic acid), more peptide bonds can form to other amino acids, extending the structure. (Figure **11.4.4**) A chain of connected amino acids is called a polypeptide. Proteins contain at least one long polypeptide chain.

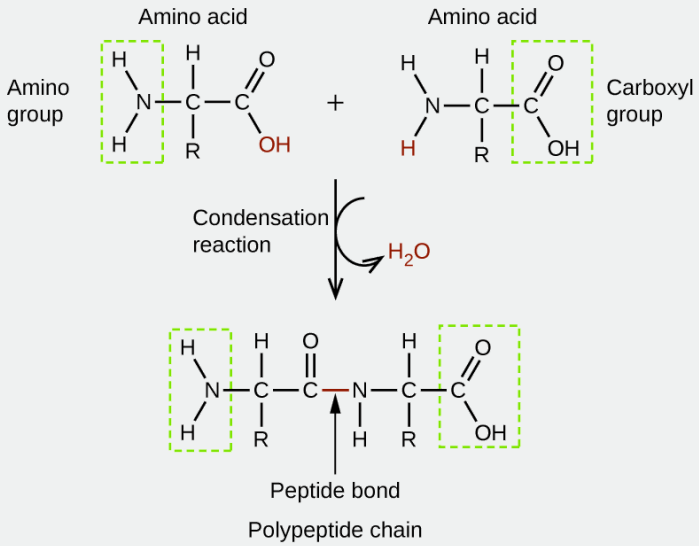


Figure **11.4.4**: This condensation reaction forms a dipeptide from two amino acids and leads to the formation of water.

Enzymes are large biological molecules, mostly composed of proteins, which are responsible for the thousands of metabolic processes that occur in living organisms. Enzymes are highly specific catalysts; they speed up the rates of certain reactions. Enzymes function by lowering the activation energy of the reaction they are catalyzing, which can dramatically increase the rate of the reaction. Most reactions catalyzed by enzymes have rates that are millions of times faster than the noncatalyzed version. Like all catalysts, enzymes are not consumed during the reactions that they catalyze. Enzymes do differ from other catalysts in how specific they are for their substrates (the molecules that an enzyme will convert into a different product). Each enzyme is only capable of speeding up one or a few very specific reactions or types of reactions. Since the function of enzymes is so specific, the lack or malfunctioning of an enzyme can lead to serious health consequences. One disease that is the result of an enzyme malfunction is phenylketonuria. In this disease, the enzyme that catalyzes the first step in the degradation of the amino acid phenylalanine is not functional (Figure **11.4.5**). Untreated, this can lead to an accumulation of phenylalanine, which can lead to intellectual disabilities.

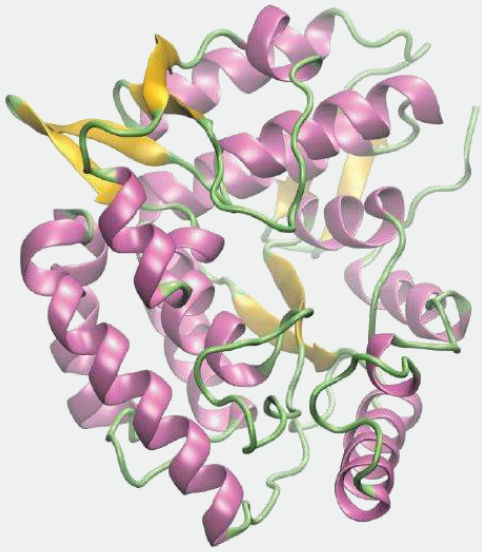


Figure **11.4.5**: A computer rendering shows the three-dimensional structure of the enzyme phenylalanine hydroxylase. In the disease phenylketonuria, a defect in the shape of phenylalanine hydroxylase causes it to lose its function in breaking down phenylalanine.

Chemistry in Everyday Life: Kevlar

Kevlar (Figure **11.4.6**) is a synthetic polymer made from two monomers 1,4-phenylene-diamine and terephthaloyl chloride (Kevlar is a registered trademark of DuPont). The material was developed by Susan Kwolek while she worked to find a replacement for steel in tires. Kwolek's work involved synthesizing polyamides and dissolving them in solvents, then spinning the resulting solution into fibers. One of her solutions proved to be quite different in initial appearance and structure. And once spun, the resulting fibers were particularly strong. From this initial discovery, Kevlar was created. The material has a high tensile strength-to-weight ratio (it is about 5 times stronger than an equal weight of steel), making it useful for many applications from bicycle tires to sails to body armor.

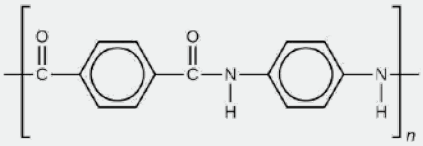


Figure **11.4.6**: This illustration shows the formula for polymeric Kevlar.

The material owes much of its strength to hydrogen bonds between polymer chains (refer back to the chapter on intermolecular interactions). These bonds form between the carbonyl group oxygen atom (which has a partial negative charge due to oxygen's electronegativity) on one monomer and the partially positively charged hydrogen atom in the N–H bond of an adjacent monomer in the polymer structure (see dashed lines in Figure **11.4.7**). There is additional strength derived from the interaction between the unhybridized *p* orbitals in the six-membered rings, called aromatic stacking.

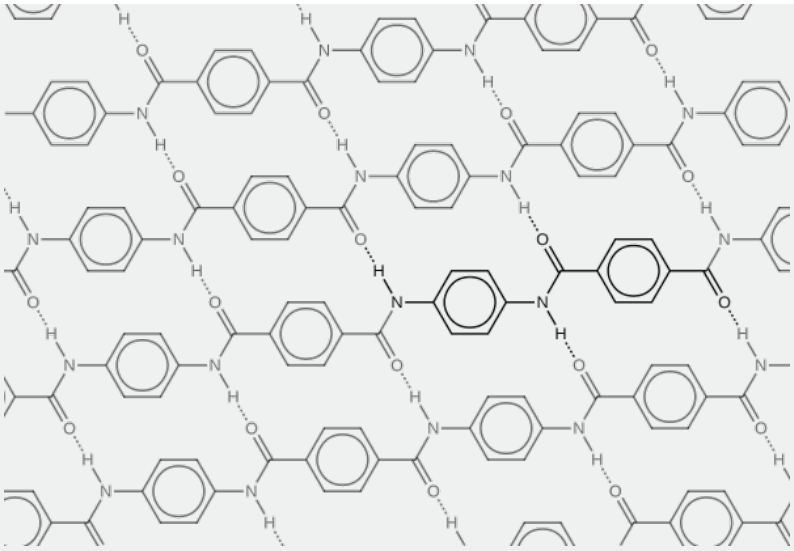


Figure **11.4.7**: The diagram shows the polymer structure of Kevlar, with hydrogen bonds between polymer chains represented by dotted lines.

Kevlar may be best known as a component of body armor, combat helmets, and face masks. Since the 1980s, the US military has used Kevlar as a component of the PASGT (personal armor system for ground troops) helmet and vest. Kevlar is also used to protect armored fighting vehicles and aircraft carriers. Civilian applications include protective gear for emergency service personnel such as body armor for police officers and heat-resistant clothing for fire fighters. Kevlar based clothing is considerably lighter and thinner than equivalent gear made from other materials (Figure **11.4.8**). Beyond Kevlar, Susan Kwolek was instrumental in the development of Nomex, a fireproof material, and was also involved in the creation of Lycra. She became just the fourth woman inducted into the National Inventors Hall of Fame, and received a number of other awards for her significant contributions to science and society.

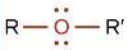
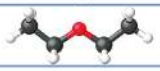
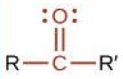
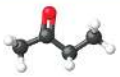
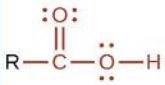
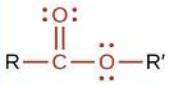
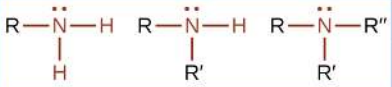
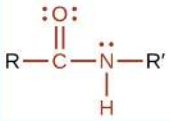


(a) (b) (c)

Figure **11.4.8**: (a) These soldiers are sorting through pieces of a Kevlar helmet that helped absorb a grenade blast. Kevlar is also used to make (b) canoes and (c) marine mooring lines. (credit a: modification of work by “Cla68”/Wikimedia Commons; credit b: modification of work by “OakleyOriginals”/Flickr; credit c: modification of work by Casey H. Kyhl)

In addition to its better-known uses, Kevlar is also often used in cryogenics for its very low thermal conductivity (along with its high strength). Kevlar maintains its high strength when cooled to the temperature of liquid nitrogen (–196 °C).

The table here summarizes the structures discussed in this chapter:

Compound Name	Structure of Compound and Functional Group (red)	Example	
		Formula	Name
alkene		C_2H_4 	ethene
alkyne		C_2H_2 	ethyne
alcohol		CH_3CH_2OH 	ethanol
ether		$(C_2H_5)_2O$ 	diethyl ether
aldehyde		CH_3CHO 	ethanal
ketone		$CH_3COCH_2CH_3$ 	methyl ethyl ketone
carboxylic acid		CH_3COOH 	acetic acid
ester		$CH_3CO_2CH_2CH_3$ 	ethyl acetate
amine		$C_2H_5NH_2$ 	ethylamine
amine			
amide		CH_3CONH_2 	acetamide

This page titled 11.4: Amines and Amides is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **20.4: Amines and Amides** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/chemistry-2e.

11.E: Exercises

Multiple Choice

11.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

12: Carbohydrates

12.1: Carbohydrates

12.2: Fischer and Haworth projections

12.3: Case Study- Tailoring Nutrition – Carbohydrates in Diabetes Care

12.E: Exercises

12: Carbohydrates is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

12.1: CARBOHYDRATES

LEARNING OBJECTIVES

By the end of this section, you will be able to do the following:

- Discuss the role of carbohydrates in cells and in the extracellular materials of animals and plants
- Explain carbohydrate classifications
- List common monosaccharides, disaccharides, and polysaccharides

Most people are familiar with carbohydrates, one type of macromolecule, especially when it comes to what we eat. To lose weight, some individuals adhere to “low-carb” diets. Athletes, in contrast, often “carb-load” before important competitions to ensure that they have enough energy to compete at a high level. Carbohydrates are, in fact, an essential part of our diet. Grains, fruits, and vegetables are all natural carbohydrate sources that provide energy to the body, particularly through glucose, a simple sugar that is a component of starch and an ingredient in many staple foods. Carbohydrates also have other important functions in humans, animals, and plants.

MOLECULAR STRUCTURES

The stoichiometric formula $(CH_2O)_n$, where n is the number of carbons in the molecule represents carbohydrates. In other words, the ratio of carbon to hydrogen to oxygen is 1:2:1 in carbohydrate molecules. This formula also explains the origin of the term “carbohydrate”: the components are carbon (“carbo”) and the components of water (hence, “hydrate”). Scientists classify carbohydrates into three subtypes: monosaccharides, disaccharides, and polysaccharides.

MONOSACCHARIDES

Monosaccharides (mono- = “one”; sacchar- = “sweet”) are simple sugars, the most common of which is glucose. In monosaccharides, the number of carbons usually ranges from three to seven. Most monosaccharide names end with the suffix -ose. If the sugar has an aldehyde group (the functional group with the structure R-CHO), it is an aldose, and if it has a ketone group (the functional group with the structure RC(=O)R'), it is a ketose. Depending on the number of carbons in the sugar, they can be trioses (three carbons), pentoses (five carbons), and/or hexoses (six carbons). Figure 3.4 illustrates monosaccharides.

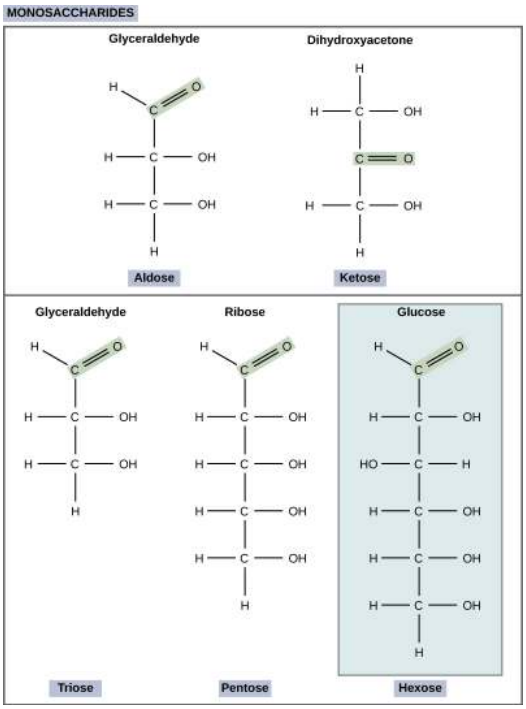


Figure 3.4 Scientists classify monosaccharides based on the position of their carbonyl group and the number of carbons in the backbone. Aldoses have a carbonyl group (indicated in green) at the end of the carbon chain, and ketoses have a carbonyl group in the middle of the carbon chain. Trioses, pentoses, and hexoses have three-, five-, and six- carbon backbones, respectively.

The chemical formula for glucose is $C_6H_{12}O_6$. In humans, glucose is an important source of energy. During cellular respiration, energy releases from glucose, and that energy helps make adenosine triphosphate (ATP). Plants synthesize glucose using carbon dioxide and water,

and glucose in turn provides energy requirements for the plant. Humans and other animals that feed on plants often obtain glucose from catabolized (cell breakdown of larger molecules) starch.

Galactose (part of lactose, or milk sugar) and fructose (found in sucrose, in fruit) are other common monosaccharides. Although glucose, galactose, and fructose all have the same chemical formula ($C_6H_{12}O_6$), they differ structurally and chemically (and are isomers) because of the different arrangement of functional groups around the asymmetric carbon. All these monosaccharides have more than one asymmetric carbon (Figure 3.5).

VISUAL CONNECTION

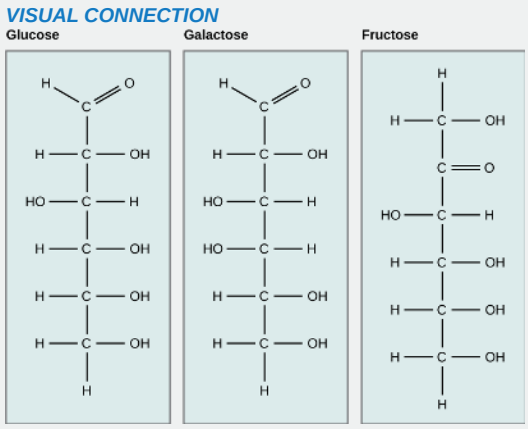


Figure 3.5 Glucose, galactose, and fructose are all hexoses. They are structural isomers, meaning they have the same chemical formula ($C_6H_{12}O_6$) but a different atom arrangement.

What kind of sugars are these, aldose or ketose?

Glucose, galactose, and fructose are isomeric monosaccharides (hexoses), meaning they have the same chemical formula but have slightly different structures. Glucose and galactose are aldoses, and fructose is a ketose.

Monosaccharides can exist as a linear chain or as ring-shaped molecules. In aqueous solutions they are usually in ring forms (Figure 3.6). Glucose in a ring form can have two different hydroxyl group arrangements (OH) around the anomeric carbon (carbon 1 that becomes asymmetric in the ring formation process). If the hydroxyl group is below carbon number 1 in the sugar, it is in the alpha (α) position, and if it is above the plane, it is in the beta (β) position.

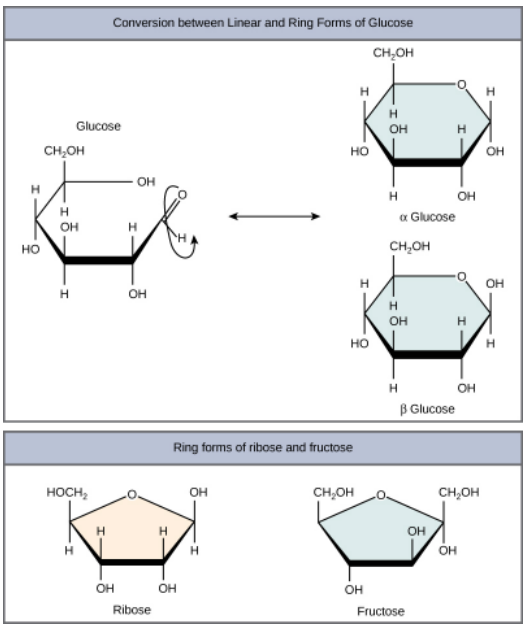


Figure 3.6 Five and six carbon monosaccharides exist in equilibrium between linear and ring forms. When the ring forms, the side chain it closes on locks into an α or β position. Fructose and ribose also form rings, although they form five-membered rings as opposed to the six-

membered ring of glucose.

DISACCHARIDES

Disaccharides (di- = “two”) form when two monosaccharides undergo a dehydration reaction (or a condensation reaction or dehydration synthesis). During this process, one monosaccharide's hydroxyl group combines with another monosaccharide's hydrogen, releasing a water molecule and forming a covalent bond. A covalent bond forms between a carbohydrate molecule and another molecule (in this case, between two monosaccharides). Scientists call this a glycosidic bond (Figure 3.7). Glycosidic bonds (or glycosidic linkages) can be an alpha or beta type. An alpha bond is formed when the OH group on the carbon-1 of the first glucose is below the ring plane, and a beta bond is formed when the OH group on the carbon-1 is above the ring plane.

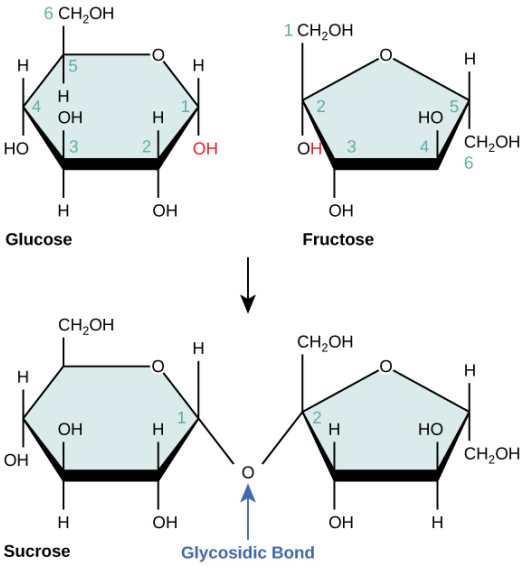


Figure 3.7 Sucrose forms when a glucose monomer and a fructose monomer join in a dehydration reaction to form a glycosidic bond. In the process, a water molecule is lost. By convention, the carbon atoms in a monosaccharide are numbered from the terminal carbon closest to the carbonyl group. In sucrose, a glycosidic linkage forms between carbon 1 in glucose and carbon 2 in fructose.

Common disaccharides include lactose, maltose, and sucrose (Figure 3.8). Lactose is a disaccharide consisting of the monomers glucose and galactose. It is naturally in milk. Maltose, or malt sugar, is a disaccharide formed by a dehydration reaction between two glucose molecules. The most common disaccharide is sucrose, or table sugar, which is comprised of glucose and fructose monomers.

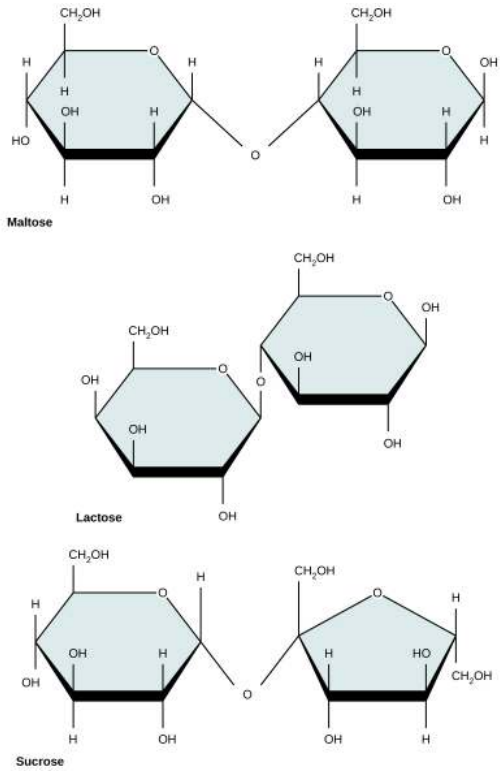


Figure 3.8 Common disaccharides include maltose (grain sugar), lactose (milk sugar), and sucrose (table sugar).

POLYSACCHARIDES

A long chain of monosaccharides linked by glycosidic bonds is a polysaccharide (poly- = “many”). The chain may be branched or unbranched, and it may contain different types of monosaccharides. The molecular weight may be 100,000 daltons or more depending on the number of joined monomers. Starch, glycogen, cellulose, and chitin are primary examples of polysaccharides.

Plants store sugars in the form of starch. In plants, an amylose and amylopectin mixture (both glucose polymers) comprise these sugars. Plants are able to synthesize glucose, and they store the excess glucose, beyond their immediate energy needs, as starch in different plant parts, including roots and seeds. The starch in the seeds provides food for the embryo as it germinates and can also act as a food source for humans and animals. Enzymes break down the starch that humans consume. For example, an amylase present in saliva catalyzes, or breaks down this starch into smaller molecules, such as maltose and glucose. The cells can then absorb the glucose.

Glucose starch comprises monomers that are joined by α 1-4 or α 1-6 glycosidic bonds. The numbers 1-4 and 1-6 refer to the carbon number of the two residues that have joined to form the bond. As Figure 3.9 illustrates, unbranched glucose monomer chains (only α 1-4 linkages) form the starch; whereas, amylopectin is a branched polysaccharide (α 1-6 linkages at the branch points).

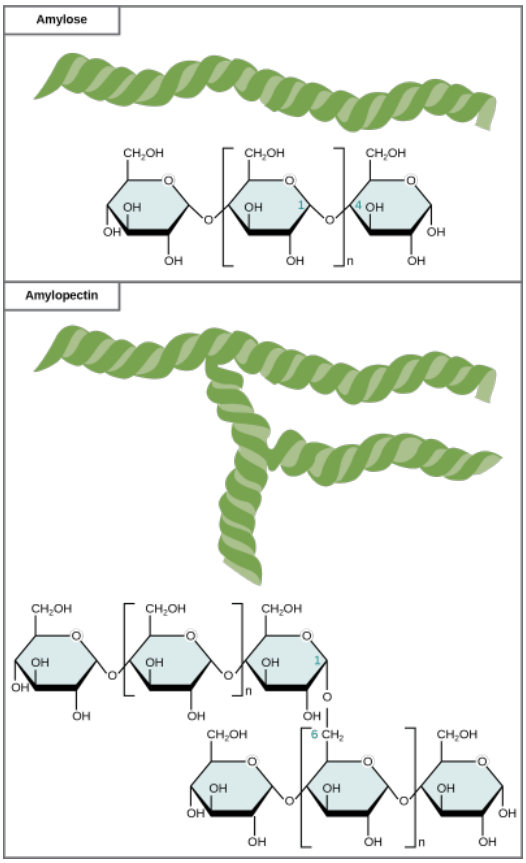


Figure 3.9 Amylose and amylopectin are two different starch forms. Unbranched glucose monomer chains comprise amylose by α 1-4 glycosidic linkages. Branched glucose monomer chains comprise amylopectin by α 1-4 and α 1-6 glycosidic linkages. Because of the way the subunits are joined, the glucose chains have a helical structure. Glycogen (not shown) is similar in structure to amylopectin but more highly branched.

Glycogen is the storage form of glucose in humans and other vertebrates and is comprised of monomers of glucose. Glycogen is the animal equivalent of starch and is a highly branched molecule usually stored in liver and muscle cells. Whenever blood glucose levels decrease, glycogen breaks down to release glucose in a process scientists call glycogenolysis.

Cellulose is the most abundant natural biopolymer. Cellulose mostly comprises a plant's cell wall. This provides the cell structural support. Wood and paper are mostly cellulosic in nature. Glucose monomers comprise cellulose that β 1-4 glycosidic bonds link (Figure 3.10).

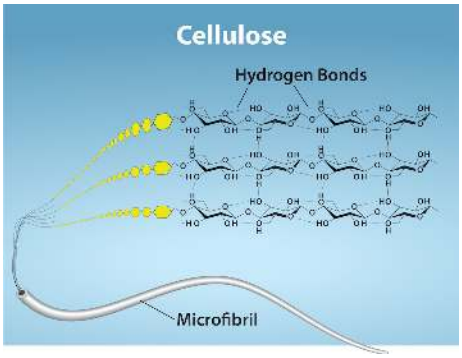


Figure 3.10 Cellulose is an organic compound composed of linear chains of hundreds to thousands of linked glucose molecules. The glucose monomers form hydrogen bonds, holding the chains firmly together side-by-side and form strong microfibrils. This rigidity is an important structural component of the cell walls found in plants. Credit: Ryan, K. Rao, A. and Hawkins, A. Department of Biology, Texas A&M University.

As Figure 3.10 shows, every other glucose monomer in cellulose is flipped over, and the monomers are packed tightly as extended long chains. This gives cellulose its rigidity and high tensile strength—which is so important to plant cells. While human digestive enzymes cannot break down the β 1-4 linkage, herbivores such as cows, koalas, and buffalos are able, with the help of the specialized flora in their stomach, to digest plant material that is rich in cellulose and use it as a food source. In some of these animals, certain species of bacteria and

protists reside in the rumen (part of the herbivore's digestive system) and secrete the enzyme cellulase. The appendix of grazing animals also contains bacteria that digest cellulose, giving it an important role in ruminants' digestive systems. Cellulases can break down cellulose into glucose monomers that animals use as an energy source. Termites are also able to break down cellulose because of the presence of other organisms in their bodies that secrete cellulases.

Carbohydrates serve various functions in different animals. Arthropods (insects, crustaceans, and others) have an outer skeleton, the exoskeleton, which protects their internal body parts (as we see in the bee in Figure 3.11). This exoskeleton is made of the biological macromolecule chitin, which is a nitrogen-containing polysaccharide. It is made of repeating N-acetyl-β-d-glucosamine units, which are a modified sugar. Chitin is also a major component of fungal cell walls. Fungi are neither animals nor plants and form a kingdom of their own in the domain Eukarya.



Figure 3.11 Insects have a hard outer exoskeleton made of chitin, a type of polysaccharide. (credit: Louise Docker)

CAREER CONNECTION

CAREER CONNECTIONS

Registered Dietitian

Obesity is a worldwide health concern, and many diseases such as diabetes and heart disease are becoming more prevalent because of obesity. This is one of the reasons why people increasingly seek out registered dietitians for advice. Registered dietitians help plan nutrition programs for individuals in various settings. They often work with patients in health care facilities, designing nutrition plans to treat and prevent diseases. For example, dietitians may teach a patient with diabetes how to manage blood sugar levels by eating the correct types and amounts of carbohydrates. Dietitians may also work in nursing homes, schools, and private practices.

To become a registered dietitian, one needs to earn at least a bachelor’s degree in dietetics, nutrition, food technology, or a related field. In addition, registered dietitians must complete a supervised internship program and pass a national exam. Those who pursue careers in dietetics take courses in nutrition, chemistry, biochemistry, biology, microbiology, and human physiology. Dietitians must become experts in the chemistry and physiology (biological functions) of food (proteins, carbohydrates, and fats).

BENEFITS OF CARBOHYDRATES

Are carbohydrates good for you? Some people believe that carbohydrates are bad and they should avoid them. Some diets completely forbid carbohydrate consumption, claiming that a low-carbohydrate diet helps people to lose weight faster. However, carbohydrates have been an important part of the human diet for thousands of years. Artifacts from ancient civilizations show the presence of wheat, rice, and corn in our ancestors’ storage areas.

As part of a well balanced diet, we should supplement carbohydrates with proteins, vitamins, and fats. Calorie-wise, a gram of carbohydrate provides 4.3 Kcal. For comparison, fats provide 9 Kcal/g, a less desirable ratio. Carbohydrates contain soluble and insoluble elements. The insoluble part, fiber, is mostly cellulose. Fiber has many uses. It promotes regular bowel movement by adding bulk, and it regulates the blood glucose consumption rate. Fiber also helps to remove excess cholesterol from the body. Fiber binds to the cholesterol in the small intestine, then attaches to the cholesterol and prevents the cholesterol particles from entering the bloodstream. Cholesterol then exits the body via the feces. Fiber-rich diets also have a protective role in reducing the occurrence of colon cancer. In addition, a meal containing whole grains and vegetables gives a feeling of fullness. As an immediate source of energy, glucose breaks down during the cellular respiration process, which produces ATP, the cell's energy currency. Without consuming carbohydrates, we reduce the availability of “instant energy”. Eliminating carbohydrates from the diet may be necessary for some people, but such a step may not be healthy for everyone.

LINK TO LEARNING

LINK TO LEARNING

For an additional perspective on carbohydrates, explore “Biomolecules: the Carbohydrates” through this interactive animation.

This page titled 12.1: Carbohydrates is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

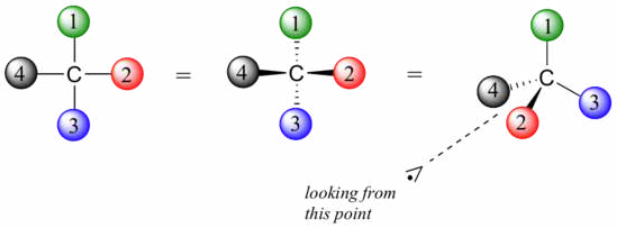
12.2: Fischer and Haworth projections

38

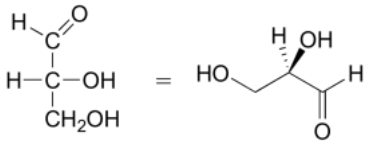
Harper College Chemistry Department

When reading the chemical and biochemical literature, you are likely to encounter several different conventions for drawing molecules in three dimensions, depending on the context of the discussion. While organic chemists prefer to use the dashed/solid wedge convention to show stereochemistry, biochemists often use drawings called **Fischer projections** and **Haworth projections** to discuss and compare the structure of sugar molecules.

Fisher projections show sugars in their open chain form. In a Fischer projection, the carbon atoms of a sugar molecule are connected vertically by solid lines, while carbon-oxygen and carbon-hydrogen bonds are shown horizontally. Stereochemical information is conveyed by a simple rule: vertical bonds point into the plane of the page, while horizontal bonds point out of the page.

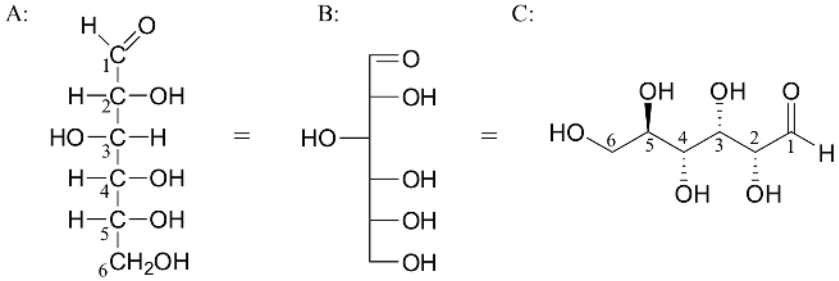


Below are two different representations of (R)-glyceraldehyde, the smallest sugar molecule (also called D -glyceraldehyde in the stereochemical nomenclature used for sugars):

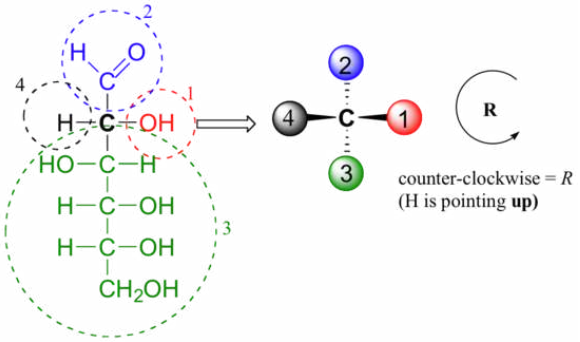


(R)-glyceraldehyde
(D-glyceraldehyde)

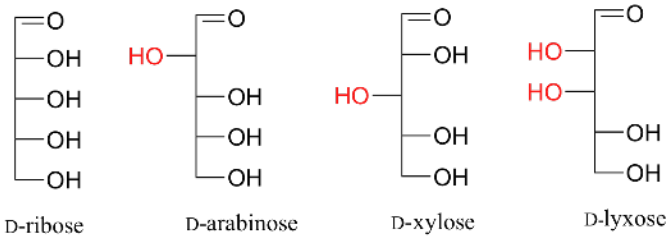
Below are three representations of the open chain form of D -glucose: in the conventional Fischer projection (A), in the “line structure” variation of the Fischer projection in which carbons and hydrogens are not shown (B), and finally in the ‘zigzag’ style (C) that is preferred by organic chemists.



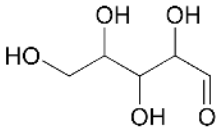
Care must be taken when ‘translating’ Fischer projection structures into’ zigzag’ format – it is easy to get the stereochemistry wrong. Probably the best way to make a translation is to simply assign *R*/*S* configurations to each stereocenter, and proceed from there. When deciding whether a stereocenter in a Fischer projection is *R* or *S*, realize that the hydrogen, in a horizontal bond, is pointing *towards* you – therefore, a counterclockwise circle means *R*, and a clockwise circle means *S* (the opposite of when the hydrogen is pointing away from you).



Fischer projections are useful when looking at many different diastereomeric sugar structures, because the eye can quickly pick out stereochemical differences according to whether a hydroxyl group is on the left or right side of the structure.

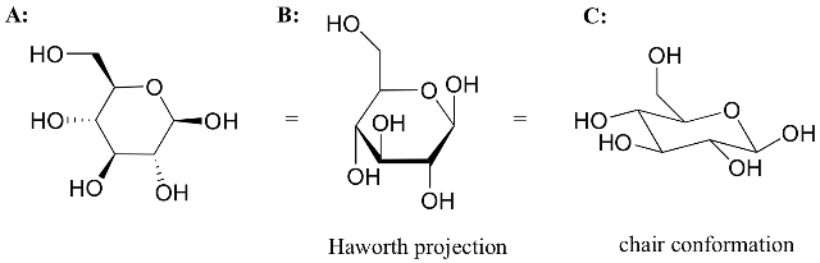


Exercise 3.24 : Draw 'zigzag' structures (using the solid/dash wedge convention to show stereochemistry) for the four sugars in the figure above. Label all stereocenters *R* or *S*. To make it easy to check your answers, draw your structures using the framework below.



Solutions to exercises

While Fischer projections are used for sugars in their open-chain form, Haworth projections are often used to depict sugars in their cyclic forms. The beta diastereomer of the cyclic form of glucose is shown below in three different depictions, with the Haworth projection in the middle.



Notice that although a Haworth projection is a convenient way to show stereochemistry, it does not provide a realistic depiction of conformation. To show *both* conformation and stereochemistry, you must draw the ring in the chair form, as in structure C above.

12.2: Fischer and Haworth projections is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

12.3: Case Study- Tailoring Nutrition – Carbohydrates in Diabetes Care

Introduction: In the daily lives of people with diabetes, carbohydrates take on a significance that goes beyond simple nutrition. As a primary energy source, the types and amounts of carbohydrates consumed can have a direct impact on blood glucose control. This case study explores the intimate role dietitians play in guiding patients through the complexities of carbohydrate management.

Scenario: Anna Roberts, a compassionate dietitian at Valley Health Hospital, is sitting down with Mr. Thompson, who has been facing the daily challenges of managing his type 2 diabetes. Together, they are embarking on a journey to adjust his diet. Anna's goal is not just to inform but to connect with Mr. Thompson on a level that reshapes his relationship with food.

The Role of Carbohydrates in the Human Body: Anna begins by walking Mr. Thompson through the basics. "Think of carbohydrates as your body's fuel," she says. She describes how the body breaks them down into sugars like glucose, which his cells use for energy, and why managing the type of 'fuel' is particularly important for his condition.

Case Study Questions:

1. **Describe the role of carbohydrates in the human body.**
2. **How can understanding carbohydrates help manage blood sugar levels?**

Hands-On Classroom Activities:

1. **Carbohydrate Analysis:** During the "Carbohydrate Analysis" activity, students will examine and quantify the carbohydrate content found in various food items and then engage in a detailed discussion about how these carbohydrates can affect blood sugar levels in the human body.

Conclusion: For Mr. Thompson, Anna's guidance turns the often-overwhelming information about diabetes into actionable and sustainable dietary choices. Her personalized approach demystifies the science of carbohydrates, making it relevant and manageable within the context of Mr. Thompson's everyday life. This case study paints a vivid picture of the crucial role dietitians like Anna play in translating the science of nutrition into personalized care plans, helping patients with diabetes take control of their health one meal at a time.

12.3: Case Study- Tailoring Nutrition – Carbohydrates in Diabetes Care is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

12.E: Exercises

Multiple Choice

1. Why do sugars usually dissolve easily in water?

    a) They have only a few hydroxyl groups

    b) They have large numbers of hydroxyl groups

    c) They have large numbers of methyl groups

    d) They have small molecular weights

2. Which of the following monosaccharides cannot form a ring structure?

    a) glucose

    b) ribose

    c) glyceraldehyde

    d) fructose

3. A carbohydrate with a C=O bond at carbon 2 would be classified as a(n)

    a) aldose

    b) ketose

    c) triose

    d) hexose

4. A carbohydrate composed of five glucose molecules would be classified as a(n)

    a) monosaccharide

    b) disaccharide

    c) oligosaccharide

    d) polysaccharide

5. Is it possible for a hydrogen bond to form between two sugar molecules?

    a) No, sugars are held together by glycosidic bonds only.

    b) Yes, the –OH group of one sugar donates a hydrogen to the –OH group on another sugar to form water.

    c) Yes, the oxygen of an –OH group can be attracted to the hydrogen on another -OH group.

    d) No, the C=O group required to form hydrogen bonds is lost when a sugar changes from a linear to a ring structure.

6. Carbohydrates are energy storage molecules because they

    a) have many different types of functional groups

    b) cannot form polymers

    c) are rich in hydrogen bonds

    d) contain accessible carbon-carbon bonds

7. To which of the following classes of sugars does glucose belong?

    a) pentose

    b) hexose

    c) tetrose

d) heptose

8. Which of the following is a disaccharide?

a) galactose

b) lactose

c) fructose

d) amylose

9. Which of the following is a monosaccharide?

a) sucrose

b) maltose

c) galactose

d) cellulose

10. Which of the following is *not* a polysaccharide?

a) extensin

b) glycogen

c) cellulose

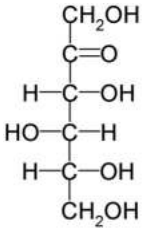
d) starch

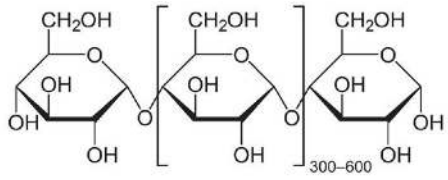
Warm-up Questions

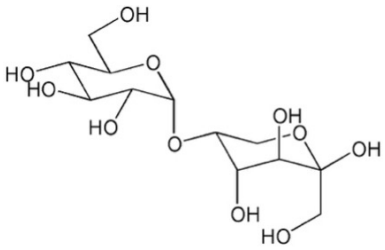
1. Polymers are synthesized by _____ reactions and broken down into monomers by _____ reactions.

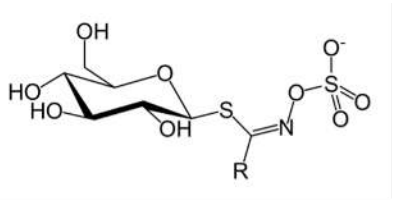
2. Isomers that differ at one of several asymmetric carbon atoms are called _____; they are called _____ when the asymmetric carbon is present in the ring form.

3-6. For each image below, indicate whether the structure is a monosaccharide, disaccharide, or polysaccharide

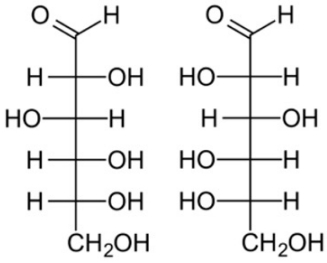
3. 

4. 

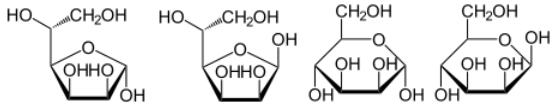
5. 

6. 

7. Identify the (D) and (L) forms of glucose and describe what distinguishes them.

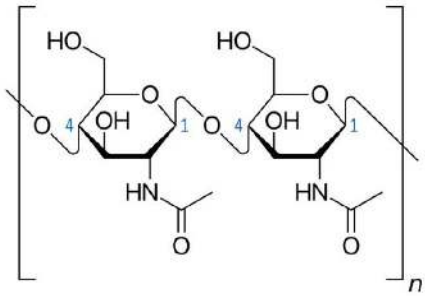


8. Identify the β-D-mannofuranose form of mannose.



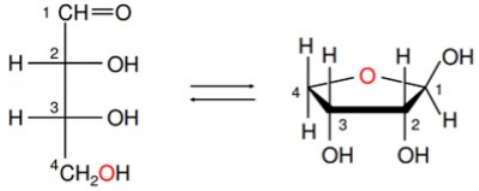
Intermediate Questions

1. Identify the monosaccharides and glycosidic linkages in this structure

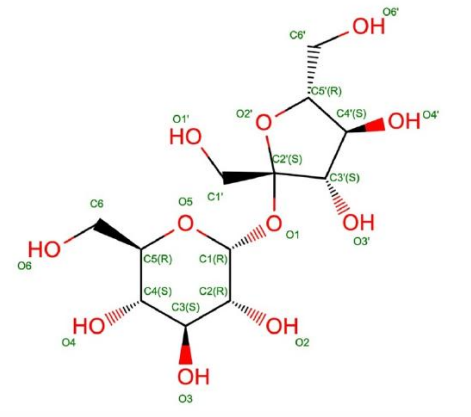


https://en.wikipedia.org/wiki/Chitin#/media/File:Haworth_projection_of_chitin.svg

2. The Fischer projection (chain) and Haworth projection (ring) for the metabolic intermediate D-erythrose are shown below. Draw a line on the Fischer projection to show the bond that is made in the ring form. Is the ring in the alpha or beta form? Is erythrose an aldose or ketose sugar?



3. This image shows a skeletal formula of the disaccharide sucrose (also known as table sugar). You can access an interactive 3D model of the molecule here. How are the two monosaccharide components of sucrose oriented with respect to each other?



https://www.rcsb.org/ligand/PRD_900003

4. Describe other ways in which the monosaccharides shown in #3 can be connected.

5-8. Indicate the structural relationship between the sugars in each pair listed below.

Example: D-glucose and D-mannose = epimers

5. D-glucose and D-fructose

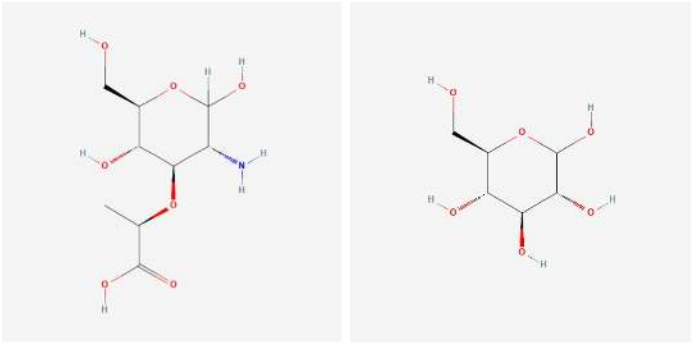
6. D-galactose and D-glucose

7. alpha-D-glucose and beta-D-glucose

8. dihydroxyacetone and D-glyceraldehyde

Challenge Questions

1. The structure of muramic acid, which is used to create cell walls in bacteria, is shown in the left panel below. How does its structure compare to that of the monosaccharide glucose, shown in the right panel?

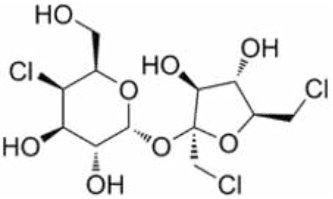


2. What are some reasons why the branched structure of glycogen is useful for energy storage?

Health-Related Questions

1. Glucose can react with other molecules in the blood to form *glycosylated* compounds. One such compound is glycosylated hemoglobin, also called hemoglobin A1c. Explain why elevated hemoglobin A1c levels are used as an indicator of diabetes.

2. The low/no-calorie sweetener (LNCS), sucralose, is a substitute for sucrose in many foods and is sold under the brand name Splenda. Sucralose is many times sweeter than table sugar but does not contribute to calorie content like sucrose does. How does the structure of sucralose compare to that of sucrose? How might these structural differences make sucralose a LNCS?



12.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

13: Lipids

13.1: Lipids

13.2: Case Study- Lipids and Heart Health - Interpreting Lipid Profiles

13.E: Exercises

13: Lipids is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

13.1: LIPIDS

LEARNING OBJECTIVES

By the end of this section, you will be able to do the following:

- Describe the four major types of lipids
- Explain the role of fats in storing energy
- Differentiate between saturated and unsaturated fatty acids
- Describe phospholipids and their role in cells
- Define the basic structure of a steroid and some steroid functions
- Explain how cholesterol helps maintain the plasma membrane's fluid nature

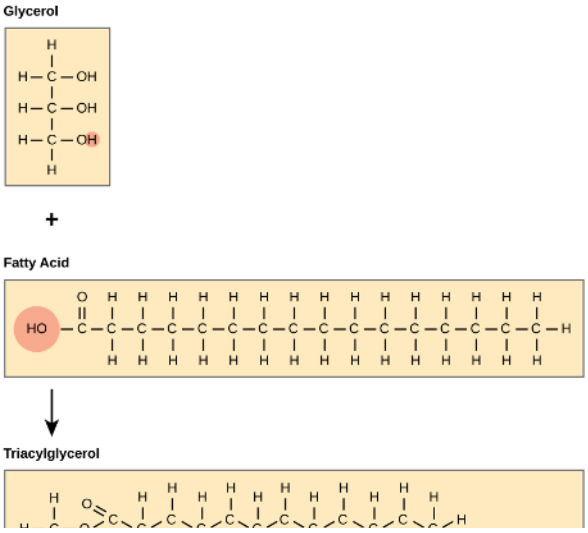
Lipids include a diverse group of compounds that are largely nonpolar in nature. This is because they are hydrocarbons that include mostly nonpolar carbon–carbon or carbon–hydrogen bonds. Non-polar molecules are hydrophobic ("water fearing"), or insoluble in water. Lipids perform many different functions in a cell. Cells store energy for long-term use in the form of fats. Lipids also provide insulation from the environment for plants and animals (Figure 3.12). For example, they help keep aquatic birds and mammals dry when forming a protective layer over fur or feathers because of their water-repellant hydrophobic nature. Lipids are also the building blocks of many hormones and are an important constituent of all cellular membranes. Lipids include fats, oils, waxes, phospholipids, and steroids.



Figure 3.12 Hydrophobic lipids in aquatic mammals' fur, such as this river otter, protect them from the elements. (credit: Ken Bosma)

FATS AND OILS

A fat molecule consists of two main components—glycerol and fatty acids. Glycerol is an organic compound (alcohol) with three carbons, five hydrogens, and three hydroxyl (OH) groups. Fatty acids have a long chain of hydrocarbons to which a carboxyl group is attached, hence the name "fatty acid." The number of carbons in the fatty acid may range from 4 to 36. The most common are those containing 12–18 carbons. In a fat molecule, the fatty acids attach to each of the glycerol molecule's three carbons with an ester bond through an oxygen atom (Figure 3.13).



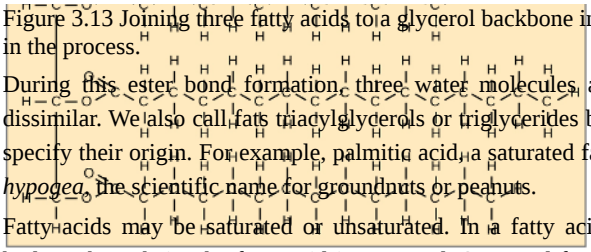


Figure 3.13 Joining three fatty acids to a glycerol backbone in a dehydration reaction forms triacylglycerol. Three water molecules release in the process.

During this ester bond formation, three water molecules are released. The three fatty acids in the triacylglycerol may be similar or dissimilar. We also call fats triacylglycerols or triglycerides because of their chemical structure. Some fatty acids have common names that specify their origin. For example, palmitic acid, a saturated fatty acid, is derived from the palm tree. Arachidic acid is derived from *Arachis hypogea*, the scientific name for groundnuts or peanuts.

Fatty acids may be saturated or unsaturated. In a fatty acid chain, if there are only single bonds between neighboring carbons in the hydrocarbon chain, the fatty acid is saturated. Saturated fatty acids are saturated with hydrogen. In other words, the number of hydrogen atoms attached to the carbon skeleton is maximized. Stearic acid is an example of a saturated fatty acid (Figure 3.14).

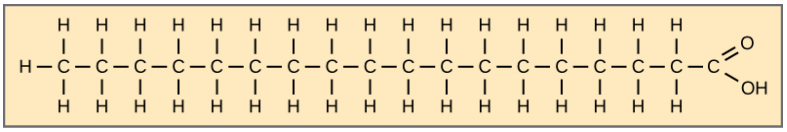


Figure 3.14 Stearic acid is a common saturated fatty acid.

When the hydrocarbon chain contains a double bond, the fatty acid is unsaturated. Oleic acid is an example of an unsaturated fatty acid (Figure 3.15).

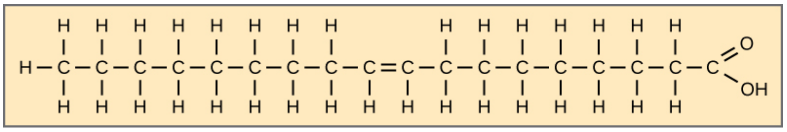


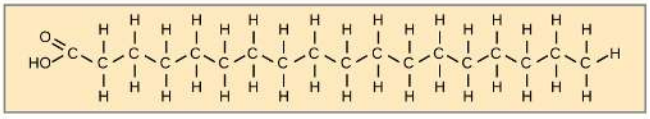
Figure 3.15 Oleic acid is a common unsaturated fatty acid.

Most unsaturated fats are liquid at room temperature. We call these oils. If there is one double bond in the molecule, then it is a monounsaturated fat (e.g., olive oil), and if there is more than one double bond, then it is a polyunsaturated fat (e.g., canola oil).

When a fatty acid has no double bonds, it is a saturated fatty acid because it is not possible to add more hydrogen to the chain's carbon atoms. A fat may contain similar or different fatty acids attached to glycerol. Long straight fatty acids with single bonds generally pack tightly and are solid at room temperature. Animal fats with stearic acid and palmitic acid (common in meat) and the fat with butyric acid (common in butter) are examples of saturated fats. Mammals store fats in specialized cells, or adipocytes, where fat globules occupy most of the cell's volume. Plants store fat or oil in many seeds and use them as a source of energy during seedling development. Unsaturated fats or oils are usually of plant origin and contain *cis* unsaturated fatty acids. *Cis* and *trans* indicate the configuration of the molecule around the double bond. If hydrogens are present in the same plane, it is a cis fat. If the hydrogen atoms are on two different planes, it is a trans fat. The *cis* double bond causes a bend or a "kink" that prevents the fatty acids from packing tightly, keeping them liquid at room temperature (Figure 3.16). Olive oil, corn oil, canola oil, and cod liver oil are examples of unsaturated fats. Unsaturated fats help to lower blood cholesterol levels; whereas, saturated fats contribute to plaque formation in the arteries.

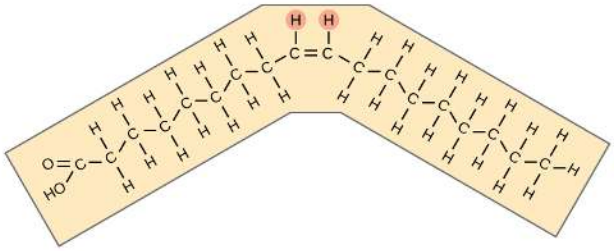
Saturated fatty acid

Stearic acid



Unsaturated fatty acids

Cis oleic acid



Trans oleic acid

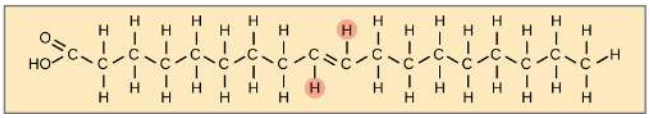


Figure 3.16 Saturated fatty acids have hydrocarbon chains connected by single bonds only. Unsaturated fatty acids have one or more double bonds. Each double bond may be in a *cis* or *trans* configuration. In the *cis* configuration, both hydrogens are on the same side of the hydrocarbon chain. In the *trans* configuration, the hydrogens are on opposite sides. A *cis* double bond causes a kink in the chain.

TRANS FATS

The food industry artificially hydrogenates oils to make them semi-solid and of a consistency desirable for many processed food products. Simply speaking, hydrogen gas is bubbled through oils to solidify them. During this hydrogenation process, double bonds of the *cis*-conformation in the hydrocarbon chain may convert to double bonds in the *trans*- conformation.

Margarine, some types of peanut butter, and shortening are examples of artificially hydrogenated trans fats. Recent studies have shown that an increase in trans fats in the human diet may lead to higher levels of low-density lipoproteins (LDL), or “bad” cholesterol, which in turn may lead to plaque deposition in the arteries, resulting in heart disease. Many fast food restaurants have recently banned using trans fats, and food labels are required to display the trans fat content.

OMEGA FATTY ACIDS

Essential fatty acids are those that the human body requires but does not synthesize. Consequently, they have to be supplemented through ingestion via the diet. Omega-3 fatty acids (like those in Figure 3.17) fall into this category and are one of only two known for humans (the other is omega-6 fatty acid). These are polyunsaturated fatty acids and are omega-3 because a double bond connects the third carbon from the hydrocarbon chain's end to its neighboring carbon.

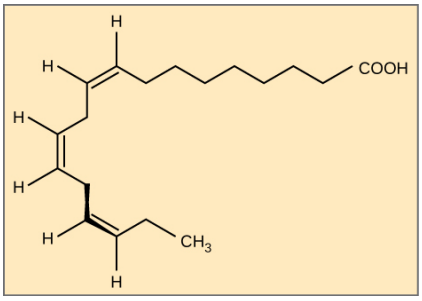


Figure 3.17 Alpha-linolenic acid is an example of an omega-3 fatty acid. It has three *cis* double bonds and, as a result, a curved shape. For clarity, the diagram does not show the carbons. Each singly bonded carbon has two hydrogens associated with it, which the diagram also does not show.

The farthest carbon away from the carboxyl group is numbered as the omega (ω) carbon, and if the double bond is between the third and fourth carbon from that end, it is an omega-3 fatty acid. Nutritionally important because the body does not make them, omega-3 fatty acids include alpha-linoleic acid (ALA), eicosapentaenoic acid (EPA), and docosahexaenoic acid (DHA), all of which are polyunsaturated. Salmon, trout, and tuna are good sources of omega-3 fatty acids. Research indicates that omega-3 fatty acids reduce the risk of sudden death

from heart attacks, lower triglycerides in the blood, decrease blood pressure, and prevent thrombosis by inhibiting blood clotting. They also reduce inflammation, and may help lower the risk of some cancers in animals.

Like carbohydrates, fats have received considerable bad publicity. It is true that eating an excess of fried foods and other “fatty” foods leads to weight gain. However, fats do have important functions. Many vitamins are fat soluble, and fats serve as a long-term storage form of fatty acids: a source of energy. They also provide insulation for the body. Therefore, we should consume “healthy” fats in moderate amounts on a regular basis.

WAXES

Wax covers some aquatic birds' feathers and some plants' leaf surfaces. Because of waxes' hydrophobic nature, they prevent water from sticking on the surface (Figure 3.18). Long fatty acid chains esterified to long-chain alcohols comprise waxes.



Figure 3.18 Lipids comprise waxy coverings on some leaves. (credit: Roger Griffith)

PHOSPHOLIPIDS

Phospholipids are major plasma membrane constituents that comprise cells' outermost layer. Like fats, they are comprised of fatty acid chains attached to a glycerol or sphingosine backbone. However, instead of three fatty acids attached as in triglycerides, there are two fatty acids forming diacylglycerol, and a modified phosphate group occupies the glycerol backbone's third carbon (Figure 3.19). A phosphate group alone attached to a diacylglycerol does not qualify as a phospholipid. It is phosphatidate (diacylglycerol 3-phosphate), the precursor of phospholipids. An alcohol modifies the phosphate group. Phosphatidylcholine and phosphatidylserine are two important phospholipids that are in plasma membranes.

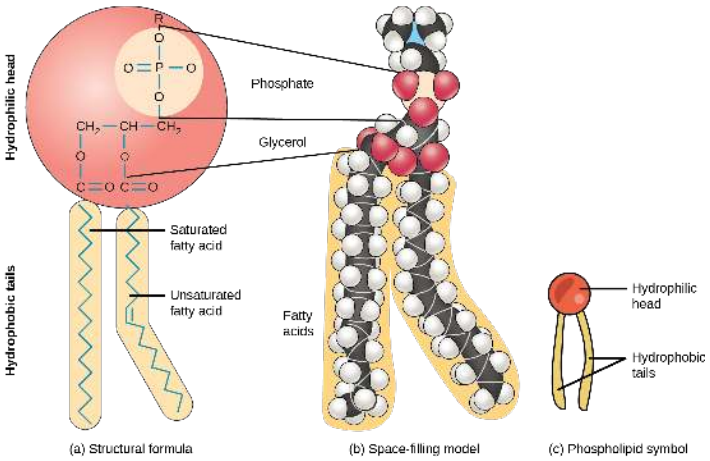


Figure 3.19 A phospholipid is a molecule with two fatty acids and a modified phosphate group attached to a glycerol backbone. Adding a charged or polar chemical group may modify the phosphate.

A phospholipid is an amphipathic molecule, meaning it has a hydrophobic and a hydrophilic part. The fatty acid chains are hydrophobic and cannot interact with water; whereas, the phosphate-containing group is hydrophilic and interacts with water (Figure 3.20).

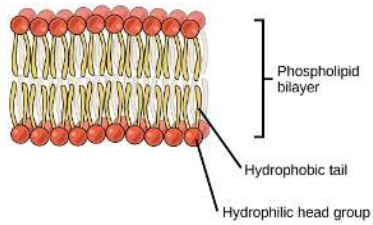


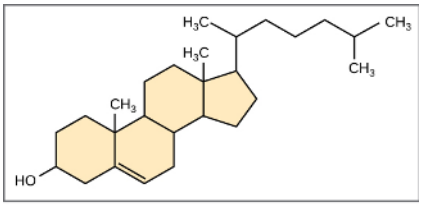
Figure 3.20 The phospholipid bilayer is the major component of all cellular membranes. The hydrophilic head groups of the phospholipids face the aqueous solution. The hydrophobic tails are sequestered in the middle of the bilayer.

The head is the hydrophilic part, and the tail contains the hydrophobic fatty acids. In a membrane, a bilayer of phospholipids forms the structure's matrix, phospholipids' fatty acid tails face inside, away from water; whereas, the phosphate group faces the outside, aqueous side (Figure 3.20).

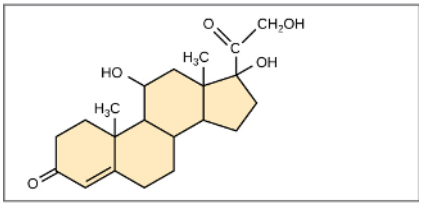
Phospholipids are responsible for the plasma membrane's dynamic nature. If a drop of phospholipids is placed in water, it spontaneously forms a structure that scientists call a micelle, where the hydrophilic phosphate heads face the outside and the fatty acids face the structure's interior.

STEROIDS

Unlike the phospholipids and fats that we discussed earlier, steroids have a fused ring structure. Although they do not resemble the other lipids, scientists group them with them because they are also hydrophobic and insoluble in water. All steroids have four linked carbon rings and several of them, like cholesterol, have a short tail (Figure 3.21). Many steroids also have the –OH functional group, which puts them in the alcohol classification (sterols).



Cholesterol



Cortisol

Figure 3.21 Four fused hydrocarbon rings comprise steroids such as cholesterol and cortisol.

Cholesterol is the most common steroid. The liver synthesizes cholesterol and is the precursor to many steroid hormones such as testosterone and estradiol, which gonads and endocrine glands secrete. It is also the precursor to Vitamin D. Cholesterol is also the precursor of bile salts, which help emulsifying fats and their subsequent absorption by cells. Although lay people often speak negatively about cholesterol, it is necessary for the body's proper functioning. Sterols (cholesterol in animal cells, phytosterol in plants) are components of the plasma membrane of cells and are found within the phospholipid bilayer.

LINK TO LEARNING

LINK TO LEARNING

For an additional perspective on lipids, watch this video about types of fat.

This page titled 13.1: Lipids is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

13.2: Case Study- Lipids and Heart Health - Interpreting Lipid Profiles

Introduction: Lipids, a diverse group of compounds including fats, oils, and cholesterol, are essential for various bodily functions but can become a health concern when present in excess. This case study explores the significance of lipids in maintaining health and how cardiologists use lipid profiles to assess the risk of cardiovascular disease (CVD) in patients.

Scenario: At Heartwise Clinic, a team of cardiologists led by Dr. Susan Clarke routinely assesses patients' risk for cardiovascular diseases by examining their lipid profiles. This involves measuring the levels of various types of cholesterol and triglycerides in the blood. Dr. Clarke is currently reviewing the lipid profile of Michael, a middle-aged patient with a family history of heart disease. She knows that these lipid levels will be instrumental in determining Michael's risk for cardiovascular events and guiding the treatment plan.

The Importance of Lipids in Health: Dr. Clarke explains to Michael that lipids serve as a major energy reserve, form cell membranes, and are precursors for important hormones. However, she also stresses that maintaining a balanced lipid profile is essential, as imbalances can lead to health issues, particularly affecting the cardiovascular system.

Case Study Questions:

1. **Explain the importance of lipids in maintaining health.**
2. **How do lipid profiles relate to cardiovascular risk?**

Hands-On Classroom Activities:

1. **Lipid Extraction:** In the "Lipid Extraction" exercise, students will perform extractions to isolate lipids from various food samples, followed by an exploration of the roles these lipids play in forming cellular structures and storing energy within organisms.

Conclusion: For patients like Michael, the lipid profile is a window into their cardiovascular health. Cardiologists like Dr. Clarke use these profiles not just to identify risks but to motivate and empower patients to make lifestyle changes or to initiate treatments that can mitigate these risks. This case study underscores the importance of understanding the dual nature of lipids as both vital to bodily functions and potential contributors to disease, illustrating the critical role they play in cardiovascular health.

13.2: Case Study- Lipids and Heart Health - Interpreting Lipid Profiles is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

13.E: Exercises

Multiple choice

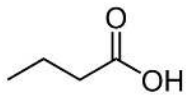
1. What are the building blocks of a phosphoglyceride, specifically phosphatidic acid?
    a. glycerol + 2 phosphate groups + 1 fatty acid
    b. glycerol + 1 phosphate group + 2 fatty acids
    c. glycerol + 1 phosphate group
    d. glycerol + 3 fatty acids
2. Which term does not describe oleic acid?
    a. polyunsaturated
    b. long-chain hydrocarbon
    c. carboxyl group
    d. carbon double bond
3. While growing some cells, you lower the temperature of the culture. What happens immediately to the membrane fluidity?
    a. Nothing happens.
    b. The membrane becomes less fluid.
    c. The membrane becomes more fluid.
    d. The membrane fluidity fluctuates back and forth from high to low.
4. The term amphipathic describes molecules that have _____.
    a. two polar regions
    b. only a single polar region
    c. both a polar and a nonpolar region
    d. no polar regions
5. Which of the following is not a polymer of numerous monomer units?
    a. carbohydrates
    b. proteins
    c. nucleic acids
    d. lipids
6. Triglycerides are composed of three fatty acids attached to a molecule of _____.
    a. glycerol
    b. phosphoric acid
    c. glucose
    d. lipid
7. Lipids are distinct from other macromolecules in that they:
    a. contain both carbon and hydrogen atoms
    b. can have both polar and non-polar components
    c. form large structures without forming covalent bonds
    d. are only found in membranes
8. The “phospho” portion of a phospholipid:
    a. is hydrophobic
    b. is hydrophilic
    c. hydrogen bonds to fatty acid chains
    d. is found on the inside of a membrane bilayer
9. A fatty acid with out carbon-carbon double bonds is considered:
    a. hydrophilic
    b. unsaturated

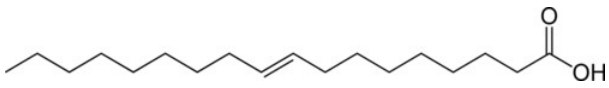
c. saturated
d. amphipathic

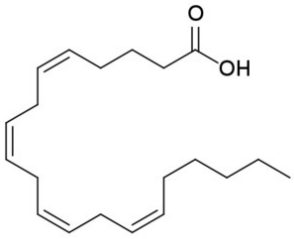
10. Which is not an example of a lipid molecule?
    a. beeswax
    b. sphingomyelin
    c. cholesterol
    d. arginine
11. The linkage between fatty acid tails and glycerol is known as an:
    a. ester bond
    b. hydrogen bond
    c. ionic bond
    d. oxygen bond
12. The presence of a “cis” double bond in a fatty acid will cause it to:
    a. undergo a condensation reaction
    b. solidify at higher temperature
    c. pack less tightly with other lipids
    d. act more like a saturated fat
13. Steroids are distinct from other lipids because they:
    a. cannot be found in membranes
    b. contain fused ring structures
    c. are insoluble in water
    d. can have polar functional groups
14. Which of the following statements is true of lipids?
    a. They contain hydrocarbon chains or rings.
    b. Cholesterol is an important phospholipid.
    c. They are more soluble in water than in alcohol.
    d. They are only used as energy-storage molecules.

Warm-up Questions

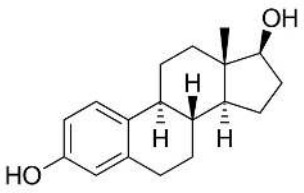
1-4. Compare the structures of the lipid molecules shown below. Use terms such as polar/nonpolar, saturated/unsaturated, and long-chain/short-chain.

1. 

2. 

3. 

4.

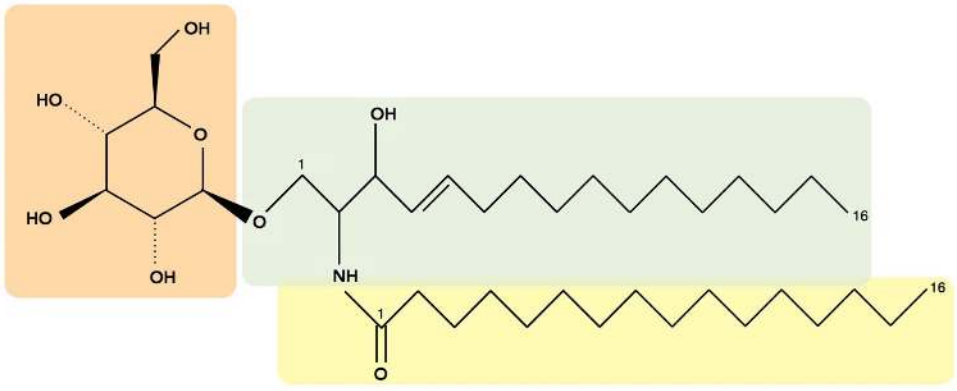


Match the following terms (1-10) to their definitions (A-J)

1. Triglyceride	A. Lipid primarily used for long-term energy storage
2. Phospholipid	B. Component of cell membranes
3. Small intestine	C. Lipid digestion begins here
4. Saturated fatty acid	D. Lipid molecule composed of a glycerol backbone and three fatty acid chains
5. Cholesterol	E. Lipid molecule with a hydrophilic head and hydrophobic tails
6. Unsaturated fatty acid	F. Lipid molecule with carbon-carbon double bonds in the fatty acid chains
7. Omega-3 fatty acid	G. Lipid molecule important for hormone synthesis
8. Lipoprotein	H. Lipid carrier proteins in the bloodstream
9. LDL and HDL	I. Lipid that can be classified as LDL or HDL
10. Chylomicrons	J. Lipid molecule with no carbon-carbon double bonds in the fatty acid chains

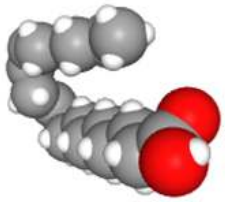
Intermediate Questions

1. Carbohydrates and lipids contain the same elements (carbon, hydrogen and oxygen) but have very different chemical properties. Explain these differences. This image shows a lipid called cerebroside. Describe its structure.
2. This image shows a lipid called cerebroside. Describe its structure.



https://u-helmich.de/bio/lexikon/C/b...rebrodid-1.jpg

3. This image shows a space-filling model of a lipid called linoleic acid. You can access an interactive 3D model of the molecule here. What chemical features are responsible for its structure?



https://pubchem.ncbi.nlm.nih.gov/compound/5280450

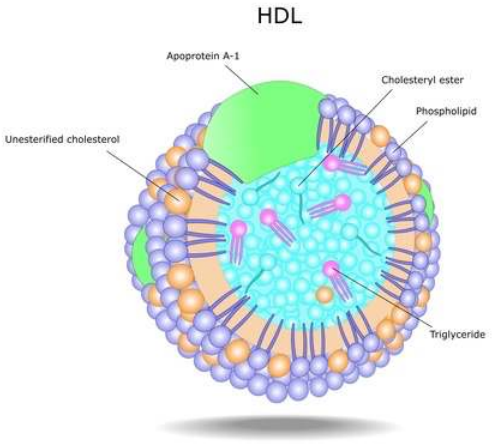
4. What are the two primary ways of packaging cholesterol? What is the purpose of each?
5. How do lipids contribute to energy storage in the body?
6. Why are triglycerides a more efficient energy storage molecule than glycogen?
7. What properties of lipids make them soluble in organic solvents?
8. What structural features determine the melting point of fatty acids?

Challenge Questions

1. How does the shape of lipid molecules affect membrane fluidity?
2. Steroid hormones such as estrogens travel through the bloodstream while bound to carrier proteins. They are recognized by receptors in the cell cytosol. Based on what you know about lipid structure and function, describe a mechanism for steroid hormone entry into cells.

Health-Related Questions

1. The image below shows a high-density lipoprotein (HDL) particle, which is part of the body's system for packaging and transporting cholesterol to the liver. Describe the structure of the HDL particle, noting the type, number and location of lipid and non-lipid components.



https://medlineplus.gov/images/PX000...SENTATION.jpeg

2. How can imbalances in lipoprotein levels such as HDL increase the risk of cardiovascular diseases such as heart attacks and stroke?

13.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

14: Proteins

14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
14.5: Case Study- Synergy in Science and Care - Protein Structures Illuminating Metabolic Disorder Management
14.6: 3D Printing Activity- Protein-Ligand Binding
14.E: Exercises

14: Proteins is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

14.1: PROPERTIES OF PROTEINS

LEARNING OBJECTIVES

By the end of this section, you will be able to do the following:

- Describe the functions proteins perform in the cell and in tissues
- Discuss the relationship between amino acids and proteins
- Explain the four levels of protein organization
- Describe the ways in which protein shape and function are linked

Proteins are one of the most abundant organic molecules in living systems and have the most diverse range of functions of all macromolecules. Proteins may be structural, regulatory, contractile, or protective. They may serve in transport, storage, or membranes; or they may be toxins or enzymes. Each cell in a living system may contain thousands of proteins, each with a unique function. Their structures, like their functions, vary greatly. They are all, however, amino acid polymers arranged in a linear sequence.

TYPES AND FUNCTIONS OF PROTEINS

Enzymes, which living cells produce, are catalysts in biochemical reactions (like digestion) and are usually complex or conjugated proteins. Each enzyme is specific for the substrate (a reactant that binds to an enzyme) upon which it acts. The enzyme may help in breakdown, rearrangement, or synthesis reactions. We call enzymes that break down their substrates catabolic enzymes. Those that build more complex molecules from their substrates are anabolic enzymes, and enzymes that affect the rate of reaction are catalytic enzymes. Note that all enzymes increase the reaction rate and, therefore, are organic catalysts. An example of an enzyme is salivary amylase, which hydrolyzes its substrate amylose, a component of starch.

Hormones are chemical-signaling molecules, usually small proteins or steroids, secreted by endocrine cells that act to control or regulate specific physiological processes, including growth, development, metabolism, and reproduction. For example, insulin is a protein hormone that helps regulate the blood glucose level. Table 3.1 lists the primary types and functions of proteins.

Protein Types and Functions

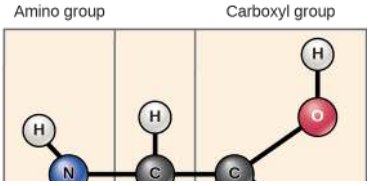
Type	Examples	Functions
Digestive Enzymes	Amylase, lipase, pepsin, trypsin	Help in food by catabolizing nutrients into monomeric units
Transport	Hemoglobin, albumin	Carry substances in the blood or lymph throughout the body
Structural	Actin, tubulin, keratin	Construct different structures, like the cytoskeleton
Hormones	Insulin, thyroxine	Coordinate different body systems' activity
Defense	Immunoglobulins	Protect the body from foreign pathogens
Contractile	Actin, myosin	Effect muscle contraction
Storage	Legume storage proteins, egg white (albumin)	Provide nourishment in early embryo development and the seedling

Table 3.1

Proteins have different shapes and molecular weights. Some proteins are globular in shape; whereas, others are fibrous in nature. For example, hemoglobin is a globular protein, but collagen, located in our skin, is a fibrous protein. Protein shape is critical to its function, and many different types of chemical bonds maintain this shape. Changes in temperature, pH, and exposure to chemicals may lead to permanent changes in the protein's shape, leading to loss of function, or denaturation. Different arrangements of the same 20 types of amino acids comprise all proteins. Two rare new amino acids were discovered recently (selenocystein and pirrolysine), and additional new discoveries may be added to the list.

AMINO ACIDS

Amino acids are the monomers that comprise proteins. Each amino acid has the same fundamental structure, which consists of a central carbon atom, or the alpha (α) carbon, bonded to an amino group (NH_2), a carboxyl group (COOH), and to a hydrogen atom. Every amino acid also has another atom or group of atoms bonded to the central atom known as the R group (Figure 3.22).



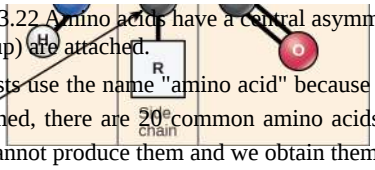


Figure 3.22 Amino acids have a central asymmetric carbon to which an amino group, a carboxyl group, a hydrogen atom, and a side chain (R group) are attached.

Scientists use the name "amino acid" because these acids contain both amino group and carboxyl-acid-group in their basic structure. As we mentioned, there are 20 common amino acids present in proteins. Nine of these are essential amino acids in humans because the human body cannot produce them and we obtain them from our diet. For each amino acid, the R group (or side chain) is different (Figure 3.23).

VISUAL CONNECTION

VISUAL CONNECTION

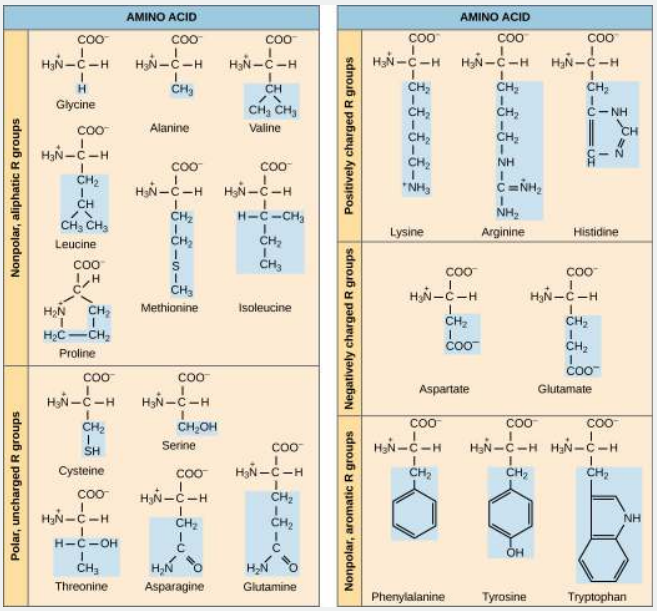


Figure 3.23 There are 20 common amino acids commonly found in proteins, each with a different R group (variant group) that determines its chemical nature.

Which categories of amino acid would you expect to find on a soluble protein's surface and which would you expect to find in the interior? What distribution of amino acids would you expect to find in a protein embedded in a lipid bilayer?

The chemical nature of the side chain determines the amino acid's nature (that is, whether it is acidic, basic, polar, or nonpolar). For example, the amino acid glycine has a hydrogen atom as the R group. Amino acids such as valine, methionine, and alanine are nonpolar or hydrophobic in nature, while amino acids such as serine, threonine, and cysteine are polar and have hydrophilic side chains. The side chains of lysine and arginine are positively charged, and therefore these amino acids are also basic amino acids. Proline has an R group that is linked to the amino group, forming a ring-like structure. Proline is an exception to the amino acid's standard structure since its amino group is not separate from the side chain (Figure 3.23).

A single upper case letter or a three-letter abbreviation represents amino acids. For example, the letter V or the three-letter symbol val represent valine. Just as some fatty acids are essential to a diet, some amino acids also are necessary. These essential amino acids in humans include isoleucine, leucine, and cysteine. Essential amino acids refer to those necessary to build proteins in the body, but not those that the body produces. Which amino acids are essential varies from organism to organism.

The sequence and the number of amino acids ultimately determine the protein's shape, size, and function. A covalent bond, or peptide bond, attaches to each amino acid, which a dehydration reaction forms. One amino acid's carboxyl group and the incoming amino acid's amino group combine, releasing a water molecule. The resulting bond is the peptide bond (Figure 3.24).

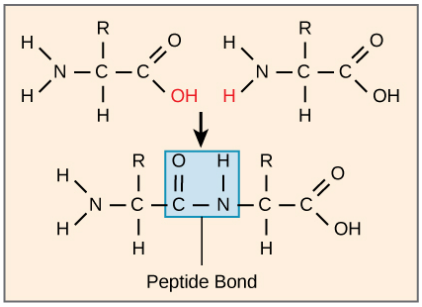


Figure 3.24 Peptide bond formation is a dehydration synthesis reaction. The carboxyl group of one amino acid is linked to the incoming amino acid's amino group. In the process, it releases a water molecule.

The products that such linkages form are peptides. As more amino acids join to this growing chain, the resulting chain is a polypeptide. Each polypeptide has a free amino group at one end. This end the N terminal, or the amino terminal, and the other end has a free carboxyl group, also the C or carboxyl terminal. While the terms polypeptide and protein are sometimes used interchangeably, a polypeptide is technically a polymer of amino acids, whereas the term protein is used for a polypeptide or polypeptides that have combined together, often have bound non-peptide prosthetic groups, have a distinct shape, and have a unique function. After protein synthesis (translation), most proteins are modified. These are known as post-translational modifications. They may undergo cleavage, phosphorylation, or may require adding other chemical groups. Only after these modifications is the protein completely functional.

LINK TO LEARNING

LINK TO LEARNING

Click through the steps of protein synthesis in this interactive tutorial.

EVOLUTION CONNECTION

EVOLUTION CONNECTION

The Evolutionary Significance of Cytochrome c

Cytochrome c is an important component of the electron transport chain, a part of cellular respiration, and it is normally located in the cellular organelle, the mitochondrion. This protein has a heme prosthetic group, and the heme's central ion alternately reduces and oxidizes during electron transfer. Because this essential protein's role in producing cellular energy is crucial, it has changed very little over millions of years. Protein sequencing has shown that there is a considerable amount of cytochrome c amino acid sequence homology among different species. In other words, we can assess evolutionary kinship by measuring the similarities or differences among various species' DNA or protein sequences.

Scientists have determined that human cytochrome c contains 104 amino acids. For each cytochrome c molecule from different organisms that scientists have sequenced to date, 37 of these amino acids appear in the same position in all cytochrome c samples. This indicates that there may have been a common ancestor. On comparing the human and chimpanzee protein sequences, scientists did not find a sequence difference. When researchers compared human and rhesus monkey sequences, the single difference was in one amino acid. In another comparison, human to yeast sequencing shows a difference in the 44th position.

PROTEIN STRUCTURE

As we discussed earlier, a protein's shape is critical to its function. For example, an enzyme can bind to a specific substrate at an active site. If this active site is altered because of local changes or changes in overall protein structure, the enzyme may be unable to bind to the substrate. To understand how the protein gets its final shape or conformation, we need to understand the four levels of protein structure: primary, secondary, tertiary, and quaternary.

PRIMARY STRUCTURE

Amino acids' unique sequence in a polypeptide chain is its primary structure. For example, the pancreatic hormone insulin has two polypeptide chains, A and B, and they are linked together by disulfide bonds. The N terminal amino acid of the A chain is glycine; whereas, the C terminal amino acid is asparagine (Figure 3.25). The amino acid sequences in the A and B chains are unique to insulin.

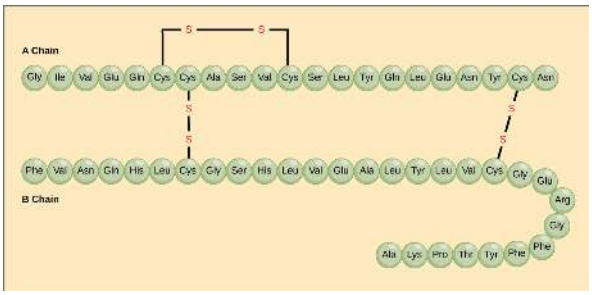


Figure 3.25 Bovine serum insulin is a protein hormone comprised of two peptide chains, A (21 amino acids long) and B (30 amino acids long). In each chain, three-letter abbreviations that represent the amino acids' names in the order they are present indicate primary structure. The amino acid cysteine (cys) has a sulfhydryl (SH) group as a side chain. Two sulfhydryl groups can react in the presence of oxygen to form a disulfide (S-S) bond. Two disulfide bonds connect the A and B chains together, and a third helps the A chain fold into the correct shape. Note that all disulfide bonds are the same length, but we have drawn them different sizes for clarity.

The gene encoding the protein ultimately determines the unique sequence for every protein. A change in nucleotide sequence of the gene's coding region may lead to adding a different amino acid to the growing polypeptide chain, causing a change in protein structure and function. In sickle cell anemia, the hemoglobin β chain (a small portion of which we show in Figure 3.26) has a single amino acid substitution, causing a change in protein structure and function. Specifically, valine in the β chain substitutes the amino acid glutamic. What is most remarkable to consider is that a hemoglobin molecule is comprised of two alpha and two beta chains that each consist of about 150 amino acids. The molecule, therefore, has about 600 amino acids. The structural difference between a normal hemoglobin molecule and a sickle cell molecule—which dramatically decreases life expectancy—is a single amino acid of the 600. What is even more remarkable is that three nucleotides each encode those 600 amino acids, and a single base change (point mutation), 1 in 1800 bases causes the mutation.

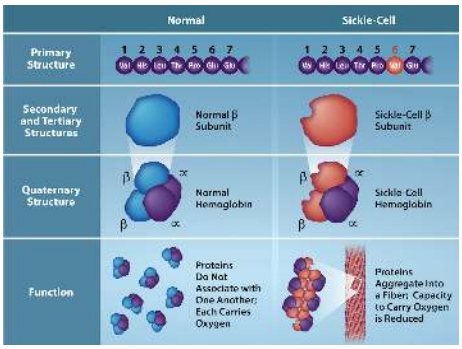


Figure 3.26 Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). .his 3.4 • Proteins 81 The beta (β)- chain of hemoglobin is 147 amino acids in length, yet a single amino acid substitution in the primary sequence leads changes in secondary, tertiary and quaternary structures and sickle cell anemia. In normal hemoglobin, the amino acid at position six is glutamate. In sickle cell hemoglobin glutamate is replaced by valine. Credit: Rao, A., Tag, A. Ryan, K. and Fletcher, S. Department of Biology, Texas A&M University.

Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). This can lead to myriad serious health problems such as breathlessness, dizziness, headaches, and abdominal pain for those affected by this disease. William Warrick Cardozo showed that sickle-cell anemia is an inherited disorder, meaning that the difference in the specific gene's encoding region is passed down from parents to children. As you will learn in the genetics unit, the inheritance of such traits is determined by a combination of genes from both parents, and these very small differences can have significant impacts on organisms.

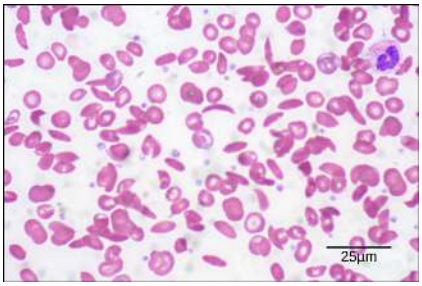


Figure 3.27 In this blood smear, visualized at 535x magnification using bright field microscopy, sickle cells are crescent shaped, while normal cells are disc-shaped. (credit: modification of work by Ed Uthman; scale-bar data from Matt Russell)

SECONDARY STRUCTURE

The local folding of the polypeptide in some regions gives rise to the secondary structure of the protein. The most common are the α-helix and β-pleated sheet structures (Figure 3.28). Both structures are held in shape by hydrogen bonds. The hydrogen bonds form between the oxygen atom in the carbonyl group in one amino acid and another amino acid that is four amino acids farther along the chain.

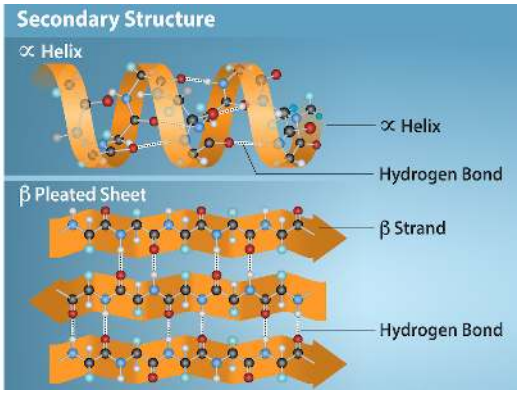


Figure 3.28 The α-helix and β-pleated sheet are secondary protein structures formed when hydrogen bonds form between the carbonyl oxygen and the amino hydrogen in the peptide backbone. Certain amino acids have a propensity to form an α-helix while others favor β-pleated sheet formation. Black = carbon, White = hydrogen, Blue = nitrogen, and Red = oxygen. Credit: Rao, A., Ryan, K. Fletcher, S. and Tag, A. Department of Biology, Texas A&M University.

Every helical turn in an alpha helix has 3.6 amino acid residues. The polypeptide's R groups (the variant groups) protrude out from the α-helix chain. In the β-pleated sheet, hydrogen bonding between atoms on the polypeptide chain's backbone form the "pleats". The R groups are attached to the carbons and extend above and below the pleat's folds. The pleated segments align parallel or antiparallel to each other, and hydrogen bonds form between the partially positive hydrogen atom in the amino group and the partially negative oxygen atom in the peptide backbone's carbonyl group. The α-helix and β-pleated sheet structures are in most globular and fibrous proteins and they play an important structural role.

TERTIARY STRUCTURE

The polypeptide's unique three-dimensional structure is its tertiary structure (Figure 3.29). This structure is in part due to chemical interactions at work on the polypeptide chain. Primarily, the interactions among R groups create the protein's complex three-dimensional tertiary structure. The nature of the R groups in the amino acids involved can counteract forming the hydrogen bonds we described for standard secondary structures. For example, R groups with like charges repel each other and those with unlike charges are attracted to each other (ionic bonds). When protein folding takes place, the nonpolar amino acids' hydrophobic R groups lie in the protein's interior; whereas, the hydrophilic R groups lie on the outside. Scientists also call the former interaction types hydrophobic interactions. Interaction between cysteine side chains forms disulfide linkages in the presence of oxygen, the only covalent bond that forms during protein folding.

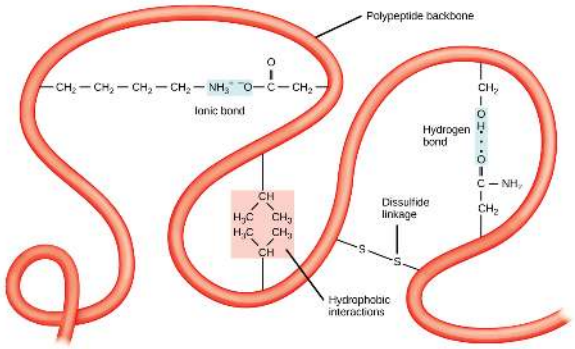


Figure 3.29 A variety of chemical interactions determine the proteins' tertiary structure. These include hydrophobic interactions, ionic bonding, hydrogen bonding, and disulfide linkages.

All of these interactions, weak and strong, determine the protein's final three-dimensional shape. When a protein loses its three-dimensional shape, it may no longer be functional.

QUATERNARY STRUCTURE

In nature, some proteins form from several polypeptides, or subunits, and the interaction of these subunits forms the quaternary structure. Weak interactions between the subunits help to stabilize the overall structure. For example, insulin (a globular protein) has a combination of hydrogen and disulfide bonds that cause it to mostly clump into a ball shape. Insulin starts out as a single polypeptide and loses some internal sequences in the presence of post-translational modification after forming the disulfide linkages that hold the remaining chains together. Silk (a fibrous protein), however, has a β-pleated sheet structure that is the result of hydrogen bonding between different chains.

Figure 3.30 illustrates the four levels of protein structure (primary, secondary, tertiary, and quaternary).

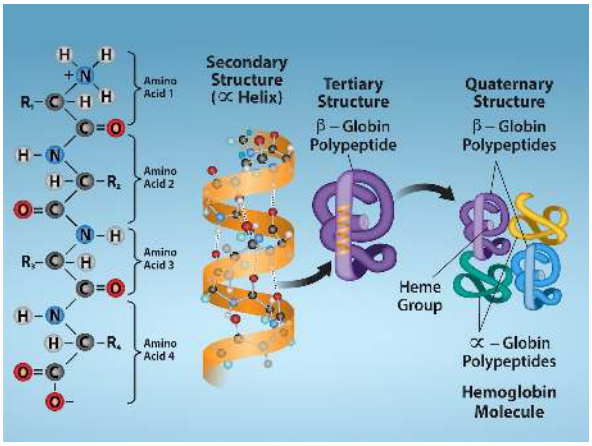


Figure 3.30 Observe the four levels of protein structure in these illustrations. Credit: Rao, A. Ryan, K. and Tag, A. Department of Biology, Texas A&M University.

DENATURATION AND PROTEIN FOLDING

Each protein has its own unique sequence and shape that chemical interactions hold together. If the protein is subject to changes in temperature, pH, or exposure to chemicals, the protein structure may change, losing its shape without losing its primary sequence in what scientists call denaturation. Denaturation is often reversible because the polypeptide's primary structure is conserved in the process if the denaturing agent is removed, allowing the protein to resume its function. Sometimes denaturation is irreversible, leading to loss of function. One example of irreversible protein denaturation is frying an egg. The albumin protein in the liquid egg white denatures when placed in a hot pan. Not all proteins denature at high temperatures. For instance, bacteria that survive in hot springs have proteins that function at temperatures close to boiling. The stomach is also very acidic, has a low pH, and denatures proteins as part of the digestion process; however, the stomach's digestive enzymes retain their activity under these conditions.

Protein folding is critical to its function. Scientists originally thought that the proteins themselves were responsible for the folding process. Only recently researchers discovered that often they receive assistance in the folding process from protein helpers, or chaperones (or chaperonins) that associate with the target protein during the folding process. They act by preventing polypeptide aggregation that comprise the complete protein structure, and they disassociate from the protein once the target protein is folded.

LINK TO LEARNING

LINK TO LEARNING

For an additional perspective on proteins, view this animation called “Biomolecules: The Proteins.”

This page titled 14.1: Properties of Proteins is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

14.2: AMINO ACIDS

LEARNING OBJECTIVES

By the end of this section, you will be able to do the following:

- Describe the functions proteins perform in the cell and in tissues
- Discuss the relationship between amino acids and proteins
- Explain the four levels of protein organization
- Describe the ways in which protein shape and function are linked

Proteins are one of the most abundant organic molecules in living systems and have the most diverse range of functions of all macromolecules. Proteins may be structural, regulatory, contractile, or protective. They may serve in transport, storage, or membranes; or they may be toxins or enzymes. Each cell in a living system may contain thousands of proteins, each with a unique function. Their structures, like their functions, vary greatly. They are all, however, amino acid polymers arranged in a linear sequence.

TYPES AND FUNCTIONS OF PROTEINS

Enzymes, which living cells produce, are catalysts in biochemical reactions (like digestion) and are usually complex or conjugated proteins. Each enzyme is specific for the substrate (a reactant that binds to an enzyme) upon which it acts. The enzyme may help in breakdown, rearrangement, or synthesis reactions. We call enzymes that break down their substrates catabolic enzymes. Those that build more complex molecules from their substrates are anabolic enzymes, and enzymes that affect the rate of reaction are catalytic enzymes. Note that all enzymes increase the reaction rate and, therefore, are organic catalysts. An example of an enzyme is salivary amylase, which hydrolyzes its substrate amylose, a component of starch.

Hormones are chemical-signaling molecules, usually small proteins or steroids, secreted by endocrine cells that act to control or regulate specific physiological processes, including growth, development, metabolism, and reproduction. For example, insulin is a protein hormone that helps regulate the blood glucose level. Table 3.1 lists the primary types and functions of proteins.

Protein Types and Functions

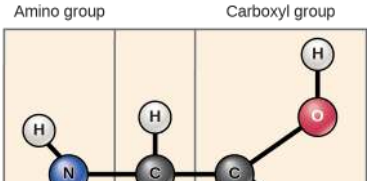
Type	Examples	Functions
Digestive Enzymes	Amylase, lipase, pepsin, trypsin	Help in food by catabolizing nutrients into monomeric units
Transport	Hemoglobin, albumin	Carry substances in the blood or lymph throughout the body
Structural	Actin, tubulin, keratin	Construct different structures, like the cytoskeleton
Hormones	Insulin, thyroxine	Coordinate different body systems' activity
Defense	Immunoglobulins	Protect the body from foreign pathogens
Contractile	Actin, myosin	Effect muscle contraction
Storage	Legume storage proteins, egg white (albumin)	Provide nourishment in early embryo development and the seedling

Table 3.1

Proteins have different shapes and molecular weights. Some proteins are globular in shape; whereas, others are fibrous in nature. For example, hemoglobin is a globular protein, but collagen, located in our skin, is a fibrous protein. Protein shape is critical to its function, and many different types of chemical bonds maintain this shape. Changes in temperature, pH, and exposure to chemicals may lead to permanent changes in the protein's shape, leading to loss of function, or denaturation. Different arrangements of the same 20 types of amino acids comprise all proteins. Two rare new amino acids were discovered recently (selenocystein and pirrolysine), and additional new discoveries may be added to the list.

AMINO ACIDS

Amino acids are the monomers that comprise proteins. Each amino acid has the same fundamental structure, which consists of a central carbon atom, or the alpha (α) carbon, bonded to an amino group (NH_2), a carboxyl group (COOH), and to a hydrogen atom. Every amino acid also has another atom or group of atoms bonded to the central atom known as the R group (Figure 3.22).



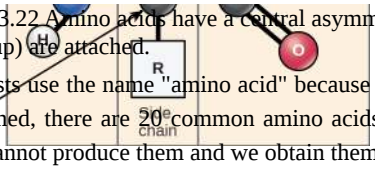


Figure 3.22 Amino acids have a central asymmetric carbon to which an amino group, a carboxyl group, a hydrogen atom, and a side chain (R group) are attached.

Scientists use the name "amino acid" because these acids contain both amino group and carboxyl-acid-group in their basic structure. As we mentioned, there are 20 common amino acids present in proteins. Nine of these are essential amino acids in humans because the human body cannot produce them and we obtain them from our diet. For each amino acid, the R group (or side chain) is different (Figure 3.23).

VISUAL CONNECTION

VISUAL CONNECTION

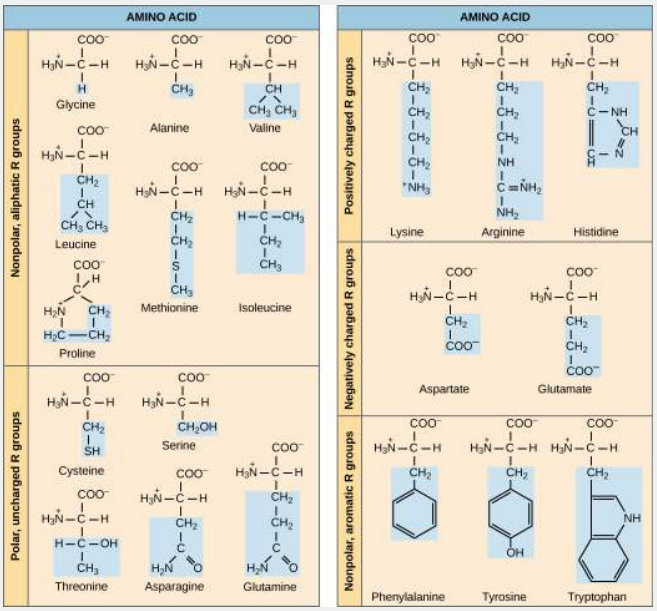


Figure 3.23 There are 20 common amino acids commonly found in proteins, each with a different R group (variant group) that determines its chemical nature.

Which categories of amino acid would you expect to find on a soluble protein's surface and which would you expect to find in the interior? What distribution of amino acids would you expect to find in a protein embedded in a lipid bilayer?

The chemical nature of the side chain determines the amino acid's nature (that is, whether it is acidic, basic, polar, or nonpolar). For example, the amino acid glycine has a hydrogen atom as the R group. Amino acids such as valine, methionine, and alanine are nonpolar or hydrophobic in nature, while amino acids such as serine, threonine, and cysteine are polar and have hydrophilic side chains. The side chains of lysine and arginine are positively charged, and therefore these amino acids are also basic amino acids. Proline has an R group that is linked to the amino group, forming a ring-like structure. Proline is an exception to the amino acid's standard structure since its amino group is not separate from the side chain (Figure 3.23).

A single upper case letter or a three-letter abbreviation represents amino acids. For example, the letter V or the three-letter symbol val represent valine. Just as some fatty acids are essential to a diet, some amino acids also are necessary. These essential amino acids in humans include isoleucine, leucine, and cysteine. Essential amino acids refer to those necessary to build proteins in the body, but not those that the body produces. Which amino acids are essential varies from organism to organism.

The sequence and the number of amino acids ultimately determine the protein's shape, size, and function. A covalent bond, or peptide bond, attaches to each amino acid, which a dehydration reaction forms. One amino acid's carboxyl group and the incoming amino acid's amino group combine, releasing a water molecule. The resulting bond is the peptide bond (Figure 3.24).

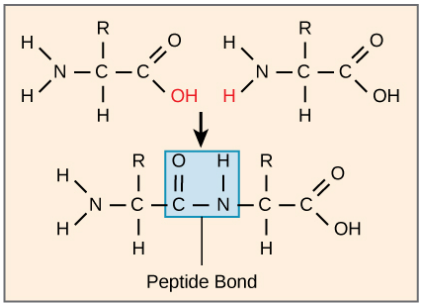


Figure 3.24 Peptide bond formation is a dehydration synthesis reaction. The carboxyl group of one amino acid is linked to the incoming amino acid's amino group. In the process, it releases a water molecule.

The products that such linkages form are peptides. As more amino acids join to this growing chain, the resulting chain is a polypeptide. Each polypeptide has a free amino group at one end. This end the N terminal, or the amino terminal, and the other end has a free carboxyl group, also the C or carboxyl terminal. While the terms polypeptide and protein are sometimes used interchangeably, a polypeptide is technically a polymer of amino acids, whereas the term protein is used for a polypeptide or polypeptides that have combined together, often have bound non-peptide prosthetic groups, have a distinct shape, and have a unique function. After protein synthesis (translation), most proteins are modified. These are known as post-translational modifications. They may undergo cleavage, phosphorylation, or may require adding other chemical groups. Only after these modifications is the protein completely functional.

LINK TO LEARNING

LINK TO LEARNING

Click through the steps of protein synthesis in this interactive tutorial.

EVOLUTION CONNECTION

EVOLUTION CONNECTION

The Evolutionary Significance of Cytochrome c

Cytochrome c is an important component of the electron transport chain, a part of cellular respiration, and it is normally located in the cellular organelle, the mitochondrion. This protein has a heme prosthetic group, and the heme's central ion alternately reduces and oxidizes during electron transfer. Because this essential protein's role in producing cellular energy is crucial, it has changed very little over millions of years. Protein sequencing has shown that there is a considerable amount of cytochrome c amino acid sequence homology among different species. In other words, we can assess evolutionary kinship by measuring the similarities or differences among various species' DNA or protein sequences.

Scientists have determined that human cytochrome c contains 104 amino acids. For each cytochrome c molecule from different organisms that scientists have sequenced to date, 37 of these amino acids appear in the same position in all cytochrome c samples. This indicates that there may have been a common ancestor. On comparing the human and chimpanzee protein sequences, scientists did not find a sequence difference. When researchers compared human and rhesus monkey sequences, the single difference was in one amino acid. In another comparison, human to yeast sequencing shows a difference in the 44th position.

PROTEIN STRUCTURE

As we discussed earlier, a protein's shape is critical to its function. For example, an enzyme can bind to a specific substrate at an active site. If this active site is altered because of local changes or changes in overall protein structure, the enzyme may be unable to bind to the substrate. To understand how the protein gets its final shape or conformation, we need to understand the four levels of protein structure: primary, secondary, tertiary, and quaternary.

PRIMARY STRUCTURE

Amino acids' unique sequence in a polypeptide chain is its primary structure. For example, the pancreatic hormone insulin has two polypeptide chains, A and B, and they are linked together by disulfide bonds. The N terminal amino acid of the A chain is glycine; whereas, the C terminal amino acid is asparagine (Figure 3.25). The amino acid sequences in the A and B chains are unique to insulin.

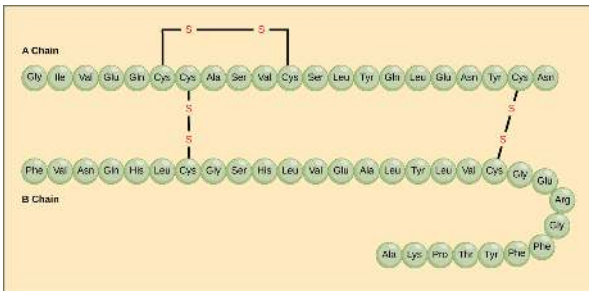


Figure 3.25 Bovine serum insulin is a protein hormone comprised of two peptide chains, A (21 amino acids long) and B (30 amino acids long). In each chain, three-letter abbreviations that represent the amino acids' names in the order they are present indicate primary structure. The amino acid cysteine (cys) has a sulfhydryl (SH) group as a side chain. Two sulfhydryl groups can react in the presence of oxygen to form a disulfide (S-S) bond. Two disulfide bonds connect the A and B chains together, and a third helps the A chain fold into the correct shape. Note that all disulfide bonds are the same length, but we have drawn them different sizes for clarity.

The gene encoding the protein ultimately determines the unique sequence for every protein. A change in nucleotide sequence of the gene's coding region may lead to adding a different amino acid to the growing polypeptide chain, causing a change in protein structure and function. In sickle cell anemia, the hemoglobin β chain (a small portion of which we show in Figure 3.26) has a single amino acid substitution, causing a change in protein structure and function. Specifically, valine in the β chain substitutes the amino acid glutamic. What is most remarkable to consider is that a hemoglobin molecule is comprised of two alpha and two beta chains that each consist of about 150 amino acids. The molecule, therefore, has about 600 amino acids. The structural difference between a normal hemoglobin molecule and a sickle cell molecule—which dramatically decreases life expectancy—is a single amino acid of the 600. What is even more remarkable is that three nucleotides each encode those 600 amino acids, and a single base change (point mutation), 1 in 1800 bases causes the mutation.

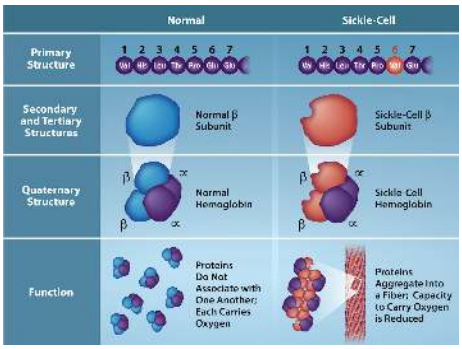


Figure 3.26 Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). .his 3.4 • Proteins 81 The beta (β)- chain of hemoglobin is 147 amino acids in length, yet a single amino acid substitution in the primary sequence leads changes in secondary, tertiary and quaternary structures and sickle cell anemia. In normal hemoglobin, the amino acid at position six is glutamate. In sickle cell hemoglobin glutamate is replaced by valine. Credit: Rao, A., Tag, A. Ryan, K. and Fletcher, S. Department of Biology, Texas A&M University.

Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). This can lead to myriad serious health problems such as breathlessness, dizziness, headaches, and abdominal pain for those affected by this disease. William Warrick Cardozo showed that sickle-cell anemia is an inherited disorder, meaning that the difference in the specific gene's encoding region is passed down from parents to children. As you will learn in the genetics unit, the inheritance of such traits is determined by a combination of genes from both parents, and these very small differences can have significant impacts on organisms.

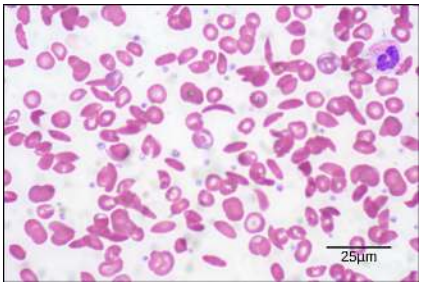


Figure 3.27 In this blood smear, visualized at 535x magnification using bright field microscopy, sickle cells are crescent shaped, while normal cells are disc-shaped. (credit: modification of work by Ed Uthman; scale-bar data from Matt Russell)

SECONDARY STRUCTURE

The local folding of the polypeptide in some regions gives rise to the secondary structure of the protein. The most common are the α-helix and β-pleated sheet structures (Figure 3.28). Both structures are held in shape by hydrogen bonds. The hydrogen bonds form between the oxygen atom in the carbonyl group in one amino acid and another amino acid that is four amino acids farther along the chain.

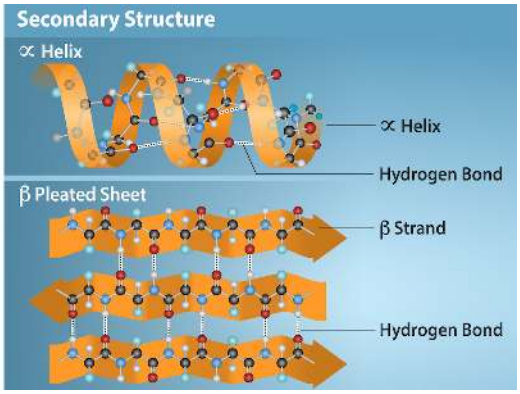


Figure 3.28 The α-helix and β-pleated sheet are secondary protein structures formed when hydrogen bonds form between the carbonyl oxygen and the amino hydrogen in the peptide backbone. Certain amino acids have a propensity to form an α-helix while others favor β-pleated sheet formation. Black = carbon, White = hydrogen, Blue = nitrogen, and Red = oxygen. Credit: Rao, A., Ryan, K. Fletcher, S. and Tag, A. Department of Biology, Texas A&M University.

Every helical turn in an alpha helix has 3.6 amino acid residues. The polypeptide's R groups (the variant groups) protrude out from the α-helix chain. In the β-pleated sheet, hydrogen bonding between atoms on the polypeptide chain's backbone form the "pleats". The R groups are attached to the carbons and extend above and below the pleat's folds. The pleated segments align parallel or antiparallel to each other, and hydrogen bonds form between the partially positive hydrogen atom in the amino group and the partially negative oxygen atom in the peptide backbone's carbonyl group. The α-helix and β-pleated sheet structures are in most globular and fibrous proteins and they play an important structural role.

TERTIARY STRUCTURE

The polypeptide's unique three-dimensional structure is its tertiary structure (Figure 3.29). This structure is in part due to chemical interactions at work on the polypeptide chain. Primarily, the interactions among R groups create the protein's complex three-dimensional tertiary structure. The nature of the R groups in the amino acids involved can counteract forming the hydrogen bonds we described for standard secondary structures. For example, R groups with like charges repel each other and those with unlike charges are attracted to each other (ionic bonds). When protein folding takes place, the nonpolar amino acids' hydrophobic R groups lie in the protein's interior; whereas, the hydrophilic R groups lie on the outside. Scientists also call the former interaction types hydrophobic interactions. Interaction between cysteine side chains forms disulfide linkages in the presence of oxygen, the only covalent bond that forms during protein folding.

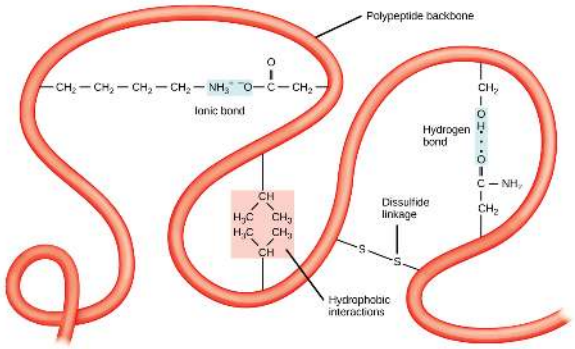


Figure 3.29 A variety of chemical interactions determine the proteins' tertiary structure. These include hydrophobic interactions, ionic bonding, hydrogen bonding, and disulfide linkages.

All of these interactions, weak and strong, determine the protein's final three-dimensional shape. When a protein loses its three-dimensional shape, it may no longer be functional.

QUATERNARY STRUCTURE

In nature, some proteins form from several polypeptides, or subunits, and the interaction of these subunits forms the quaternary structure. Weak interactions between the subunits help to stabilize the overall structure. For example, insulin (a globular protein) has a combination of hydrogen and disulfide bonds that cause it to mostly clump into a ball shape. Insulin starts out as a single polypeptide and loses some internal sequences in the presence of post-translational modification after forming the disulfide linkages that hold the remaining chains together. Silk (a fibrous protein), however, has a β-pleated sheet structure that is the result of hydrogen bonding between different chains.

Figure 3.30 illustrates the four levels of protein structure (primary, secondary, tertiary, and quaternary).

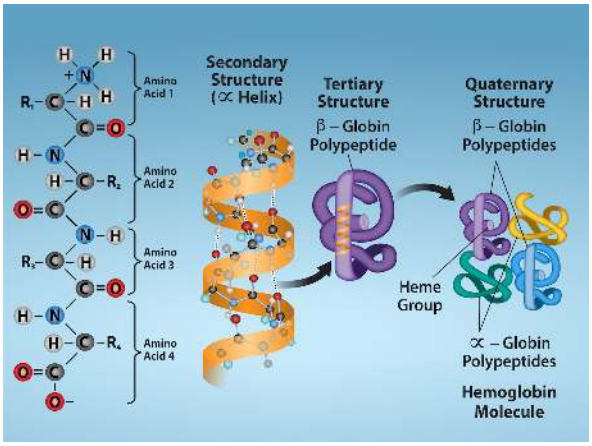


Figure 3.30 Observe the four levels of protein structure in these illustrations. Credit: Rao, A. Ryan, K. and Tag, A. Department of Biology, Texas A&M University.

DENATURATION AND PROTEIN FOLDING

Each protein has its own unique sequence and shape that chemical interactions hold together. If the protein is subject to changes in temperature, pH, or exposure to chemicals, the protein structure may change, losing its shape without losing its primary sequence in what scientists call denaturation. Denaturation is often reversible because the polypeptide's primary structure is conserved in the process if the denaturing agent is removed, allowing the protein to resume its function. Sometimes denaturation is irreversible, leading to loss of function. One example of irreversible protein denaturation is frying an egg. The albumin protein in the liquid egg white denatures when placed in a hot pan. Not all proteins denature at high temperatures. For instance, bacteria that survive in hot springs have proteins that function at temperatures close to boiling. The stomach is also very acidic, has a low pH, and denatures proteins as part of the digestion process; however, the stomach's digestive enzymes retain their activity under these conditions.

Protein folding is critical to its function. Scientists originally thought that the proteins themselves were responsible for the folding process. Only recently researchers discovered that often they receive assistance in the folding process from protein helpers, or chaperones (or chaperonins) that associate with the target protein during the folding process. They act by preventing polypeptide aggregation that comprise the complete protein structure, and they disassociate from the protein once the target protein is folded.

LINK TO LEARNING

LINK TO LEARNING

For an additional perspective on proteins, view this animation called “Biomolecules: The Proteins.”

This page titled 14.2: Amino Acids is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

14.3: PRIMARY STRUCTURE- PEPTIDES

LEARNING OBJECTIVES

By the end of this section, you will be able to do the following:

- Describe the functions proteins perform in the cell and in tissues
- Discuss the relationship between amino acids and proteins
- Explain the four levels of protein organization
- Describe the ways in which protein shape and function are linked

Proteins are one of the most abundant organic molecules in living systems and have the most diverse range of functions of all macromolecules. Proteins may be structural, regulatory, contractile, or protective. They may serve in transport, storage, or membranes; or they may be toxins or enzymes. Each cell in a living system may contain thousands of proteins, each with a unique function. Their structures, like their functions, vary greatly. They are all, however, amino acid polymers arranged in a linear sequence.

TYPES AND FUNCTIONS OF PROTEINS

Enzymes, which living cells produce, are catalysts in biochemical reactions (like digestion) and are usually complex or conjugated proteins. Each enzyme is specific for the substrate (a reactant that binds to an enzyme) upon which it acts. The enzyme may help in breakdown, rearrangement, or synthesis reactions. We call enzymes that break down their substrates catabolic enzymes. Those that build more complex molecules from their substrates are anabolic enzymes, and enzymes that affect the rate of reaction are catalytic enzymes. Note that all enzymes increase the reaction rate and, therefore, are organic catalysts. An example of an enzyme is salivary amylase, which hydrolyzes its substrate amylose, a component of starch.

Hormones are chemical-signaling molecules, usually small proteins or steroids, secreted by endocrine cells that act to control or regulate specific physiological processes, including growth, development, metabolism, and reproduction. For example, insulin is a protein hormone that helps regulate the blood glucose level. Table 3.1 lists the primary types and functions of proteins.

Protein Types and Functions

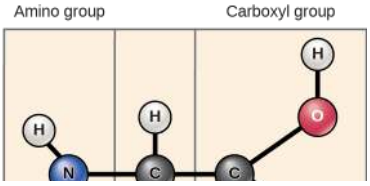
Type	Examples	Functions
Digestive Enzymes	Amylase, lipase, pepsin, trypsin	Help in food by catabolizing nutrients into monomeric units
Transport	Hemoglobin, albumin	Carry substances in the blood or lymph throughout the body
Structural	Actin, tubulin, keratin	Construct different structures, like the cytoskeleton
Hormones	Insulin, thyroxine	Coordinate different body systems' activity
Defense	Immunoglobulins	Protect the body from foreign pathogens
Contractile	Actin, myosin	Effect muscle contraction
Storage	Legume storage proteins, egg white (albumin)	Provide nourishment in early embryo development and the seedling

Table 3.1

Proteins have different shapes and molecular weights. Some proteins are globular in shape; whereas, others are fibrous in nature. For example, hemoglobin is a globular protein, but collagen, located in our skin, is a fibrous protein. Protein shape is critical to its function, and many different types of chemical bonds maintain this shape. Changes in temperature, pH, and exposure to chemicals may lead to permanent changes in the protein's shape, leading to loss of function, or denaturation. Different arrangements of the same 20 types of amino acids comprise all proteins. Two rare new amino acids were discovered recently (selenocystein and pirrolysine), and additional new discoveries may be added to the list.

AMINO ACIDS

Amino acids are the monomers that comprise proteins. Each amino acid has the same fundamental structure, which consists of a central carbon atom, or the alpha (α) carbon, bonded to an amino group (NH_2), a carboxyl group (COOH), and to a hydrogen atom. Every amino acid also has another atom or group of atoms bonded to the central atom known as the R group (Figure 3.22).



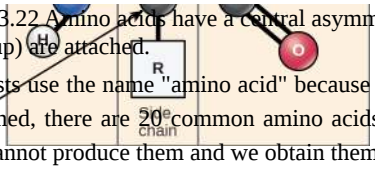


Figure 3.22 Amino acids have a central asymmetric carbon to which an amino group, a carboxyl group, a hydrogen atom, and a side chain (R group) are attached.

Scientists use the name "amino acid" because these acids contain both amino group and carboxyl-acid-group in their basic structure. As we mentioned, there are 20 common amino acids present in proteins. Nine of these are essential amino acids in humans because the human body cannot produce them and we obtain them from our diet. For each amino acid, the R group (or side chain) is different (Figure 3.23).

VISUAL CONNECTION

VISUAL CONNECTION

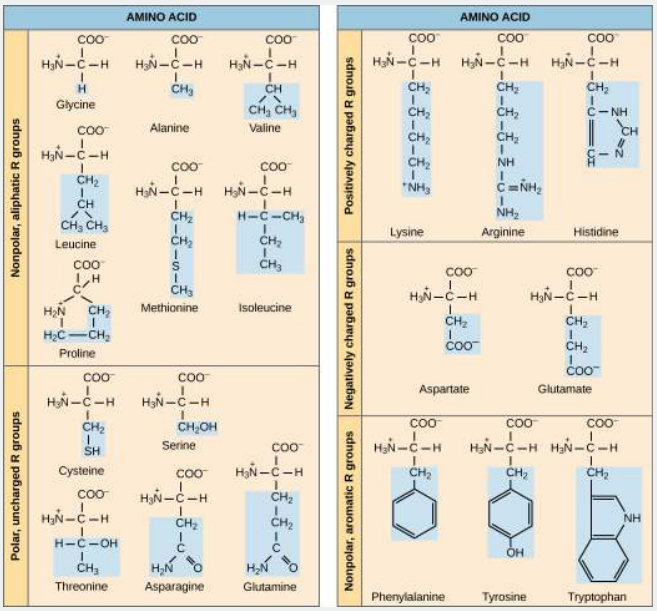


Figure 3.23 There are 20 common amino acids commonly found in proteins, each with a different R group (variant group) that determines its chemical nature.

Which categories of amino acid would you expect to find on a soluble protein's surface and which would you expect to find in the interior? What distribution of amino acids would you expect to find in a protein embedded in a lipid bilayer?

The chemical nature of the side chain determines the amino acid's nature (that is, whether it is acidic, basic, polar, or nonpolar). For example, the amino acid glycine has a hydrogen atom as the R group. Amino acids such as valine, methionine, and alanine are nonpolar or hydrophobic in nature, while amino acids such as serine, threonine, and cysteine are polar and have hydrophilic side chains. The side chains of lysine and arginine are positively charged, and therefore these amino acids are also basic amino acids. Proline has an R group that is linked to the amino group, forming a ring-like structure. Proline is an exception to the amino acid's standard structure since its amino group is not separate from the side chain (Figure 3.23).

A single upper case letter or a three-letter abbreviation represents amino acids. For example, the letter V or the three-letter symbol val represent valine. Just as some fatty acids are essential to a diet, some amino acids also are necessary. These essential amino acids in humans include isoleucine, leucine, and cysteine. Essential amino acids refer to those necessary to build proteins in the body, but not those that the body produces. Which amino acids are essential varies from organism to organism.

The sequence and the number of amino acids ultimately determine the protein's shape, size, and function. A covalent bond, or peptide bond, attaches to each amino acid, which a dehydration reaction forms. One amino acid's carboxyl group and the incoming amino acid's amino group combine, releasing a water molecule. The resulting bond is the peptide bond (Figure 3.24).

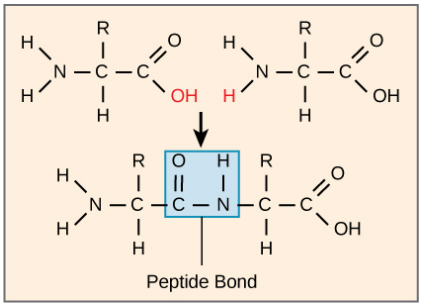


Figure 3.24 Peptide bond formation is a dehydration synthesis reaction. The carboxyl group of one amino acid is linked to the incoming amino acid's amino group. In the process, it releases a water molecule.

The products that such linkages form are peptides. As more amino acids join to this growing chain, the resulting chain is a polypeptide. Each polypeptide has a free amino group at one end. This end the N terminal, or the amino terminal, and the other end has a free carboxyl group, also the C or carboxyl terminal. While the terms polypeptide and protein are sometimes used interchangeably, a polypeptide is technically a polymer of amino acids, whereas the term protein is used for a polypeptide or polypeptides that have combined together, often have bound non-peptide prosthetic groups, have a distinct shape, and have a unique function. After protein synthesis (translation), most proteins are modified. These are known as post-translational modifications. They may undergo cleavage, phosphorylation, or may require adding other chemical groups. Only after these modifications is the protein completely functional.

LINK TO LEARNING

LINK TO LEARNING

Click through the steps of protein synthesis in this interactive tutorial.

EVOLUTION CONNECTION

EVOLUTION CONNECTION

The Evolutionary Significance of Cytochrome c

Cytochrome c is an important component of the electron transport chain, a part of cellular respiration, and it is normally located in the cellular organelle, the mitochondrion. This protein has a heme prosthetic group, and the heme's central ion alternately reduces and oxidizes during electron transfer. Because this essential protein's role in producing cellular energy is crucial, it has changed very little over millions of years. Protein sequencing has shown that there is a considerable amount of cytochrome c amino acid sequence homology among different species. In other words, we can assess evolutionary kinship by measuring the similarities or differences among various species' DNA or protein sequences.

Scientists have determined that human cytochrome c contains 104 amino acids. For each cytochrome c molecule from different organisms that scientists have sequenced to date, 37 of these amino acids appear in the same position in all cytochrome c samples. This indicates that there may have been a common ancestor. On comparing the human and chimpanzee protein sequences, scientists did not find a sequence difference. When researchers compared human and rhesus monkey sequences, the single difference was in one amino acid. In another comparison, human to yeast sequencing shows a difference in the 44th position.

PROTEIN STRUCTURE

As we discussed earlier, a protein's shape is critical to its function. For example, an enzyme can bind to a specific substrate at an active site. If this active site is altered because of local changes or changes in overall protein structure, the enzyme may be unable to bind to the substrate. To understand how the protein gets its final shape or conformation, we need to understand the four levels of protein structure: primary, secondary, tertiary, and quaternary.

PRIMARY STRUCTURE

Amino acids' unique sequence in a polypeptide chain is its primary structure. For example, the pancreatic hormone insulin has two polypeptide chains, A and B, and they are linked together by disulfide bonds. The N terminal amino acid of the A chain is glycine; whereas, the C terminal amino acid is asparagine (Figure 3.25). The amino acid sequences in the A and B chains are unique to insulin.

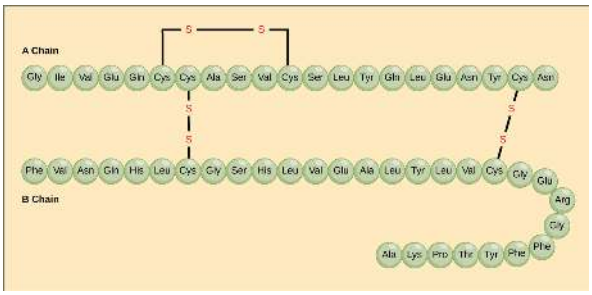


Figure 3.25 Bovine serum insulin is a protein hormone comprised of two peptide chains, A (21 amino acids long) and B (30 amino acids long). In each chain, three-letter abbreviations that represent the amino acids' names in the order they are present indicate primary structure. The amino acid cysteine (cys) has a sulfhydryl (SH) group as a side chain. Two sulfhydryl groups can react in the presence of oxygen to form a disulfide (S-S) bond. Two disulfide bonds connect the A and B chains together, and a third helps the A chain fold into the correct shape. Note that all disulfide bonds are the same length, but we have drawn them different sizes for clarity.

The gene encoding the protein ultimately determines the unique sequence for every protein. A change in nucleotide sequence of the gene's coding region may lead to adding a different amino acid to the growing polypeptide chain, causing a change in protein structure and function. In sickle cell anemia, the hemoglobin β chain (a small portion of which we show in Figure 3.26) has a single amino acid substitution, causing a change in protein structure and function. Specifically, valine in the β chain substitutes the amino acid glutamic. What is most remarkable to consider is that a hemoglobin molecule is comprised of two alpha and two beta chains that each consist of about 150 amino acids. The molecule, therefore, has about 600 amino acids. The structural difference between a normal hemoglobin molecule and a sickle cell molecule—which dramatically decreases life expectancy—is a single amino acid of the 600. What is even more remarkable is that three nucleotides each encode those 600 amino acids, and a single base change (point mutation), 1 in 1800 bases causes the mutation.

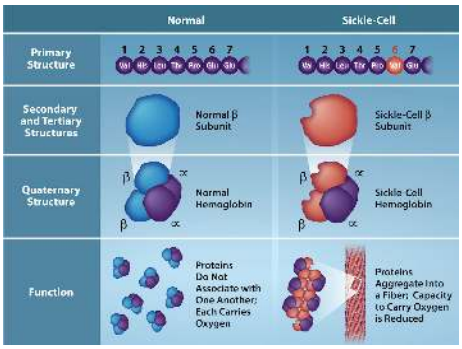


Figure 3.26 Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). .his 3.4 • Proteins 81 The beta (β)- chain of hemoglobin is 147 amino acids in length, yet a single amino acid substitution in the primary sequence leads changes in secondary, tertiary and quaternary structures and sickle cell anemia. In normal hemoglobin, the amino acid at position six is glutamate. In sickle cell hemoglobin glutamate is replaced by valine. Credit: Rao, A., Tag, A. Ryan, K. and Fletcher, S. Department of Biology, Texas A&M University.

Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). This can lead to myriad serious health problems such as breathlessness, dizziness, headaches, and abdominal pain for those affected by this disease. William Warrick Cardozo showed that sickle-cell anemia is an inherited disorder, meaning that the difference in the specific gene's encoding region is passed down from parents to children. As you will learn in the genetics unit, the inheritance of such traits is determined by a combination of genes from both parents, and these very small differences can have significant impacts on organisms.

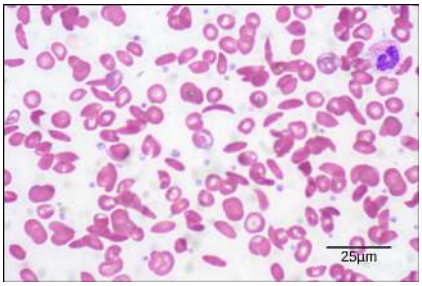


Figure 3.27 In this blood smear, visualized at 535x magnification using bright field microscopy, sickle cells are crescent shaped, while normal cells are disc-shaped. (credit: modification of work by Ed Uthman; scale-bar data from Matt Russell)

SECONDARY STRUCTURE

The local folding of the polypeptide in some regions gives rise to the secondary structure of the protein. The most common are the α-helix and β-pleated sheet structures (Figure 3.28). Both structures are held in shape by hydrogen bonds. The hydrogen bonds form between the oxygen atom in the carbonyl group in one amino acid and another amino acid that is four amino acids farther along the chain.

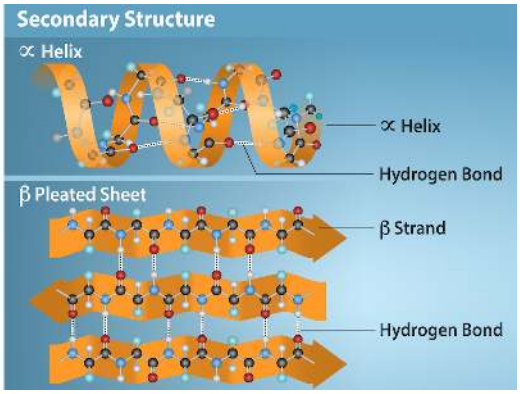


Figure 3.28 The α-helix and β-pleated sheet are secondary protein structures formed when hydrogen bonds form between the carbonyl oxygen and the amino hydrogen in the peptide backbone. Certain amino acids have a propensity to form an α-helix while others favor β-pleated sheet formation. Black = carbon, White = hydrogen, Blue = nitrogen, and Red = oxygen. Credit: Rao, A., Ryan, K. Fletcher, S. and Tag, A. Department of Biology, Texas A&M University.

Every helical turn in an alpha helix has 3.6 amino acid residues. The polypeptide's R groups (the variant groups) protrude out from the α-helix chain. In the β-pleated sheet, hydrogen bonding between atoms on the polypeptide chain's backbone form the "pleats". The R groups are attached to the carbons and extend above and below the pleat's folds. The pleated segments align parallel or antiparallel to each other, and hydrogen bonds form between the partially positive hydrogen atom in the amino group and the partially negative oxygen atom in the peptide backbone's carbonyl group. The α-helix and β-pleated sheet structures are in most globular and fibrous proteins and they play an important structural role.

TERTIARY STRUCTURE

The polypeptide's unique three-dimensional structure is its tertiary structure (Figure 3.29). This structure is in part due to chemical interactions at work on the polypeptide chain. Primarily, the interactions among R groups create the protein's complex three-dimensional tertiary structure. The nature of the R groups in the amino acids involved can counteract forming the hydrogen bonds we described for standard secondary structures. For example, R groups with like charges repel each other and those with unlike charges are attracted to each other (ionic bonds). When protein folding takes place, the nonpolar amino acids' hydrophobic R groups lie in the protein's interior; whereas, the hydrophilic R groups lie on the outside. Scientists also call the former interaction types hydrophobic interactions. Interaction between cysteine side chains forms disulfide linkages in the presence of oxygen, the only covalent bond that forms during protein folding.

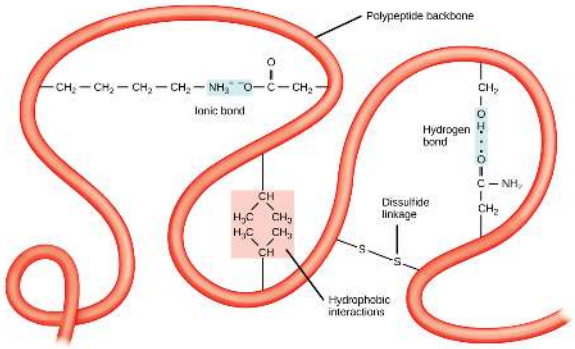


Figure 3.29 A variety of chemical interactions determine the proteins' tertiary structure. These include hydrophobic interactions, ionic bonding, hydrogen bonding, and disulfide linkages.

All of these interactions, weak and strong, determine the protein's final three-dimensional shape. When a protein loses its three-dimensional shape, it may no longer be functional.

QUATERNARY STRUCTURE

In nature, some proteins form from several polypeptides, or subunits, and the interaction of these subunits forms the quaternary structure. Weak interactions between the subunits help to stabilize the overall structure. For example, insulin (a globular protein) has a combination of hydrogen and disulfide bonds that cause it to mostly clump into a ball shape. Insulin starts out as a single polypeptide and loses some internal sequences in the presence of post-translational modification after forming the disulfide linkages that hold the remaining chains together. Silk (a fibrous protein), however, has a β-pleated sheet structure that is the result of hydrogen bonding between different chains.

Figure 3.30 illustrates the four levels of protein structure (primary, secondary, tertiary, and quaternary).

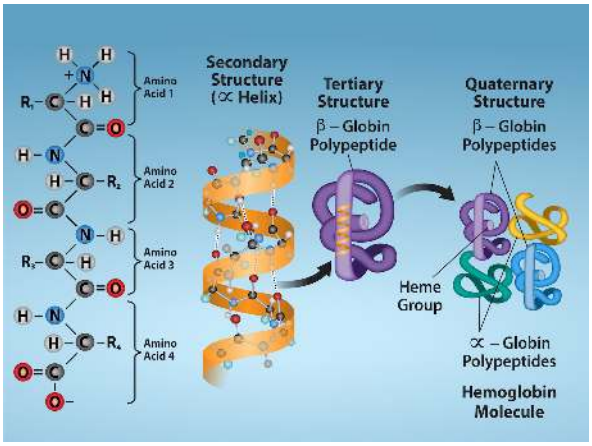


Figure 3.30 Observe the four levels of protein structure in these illustrations. Credit: Rao, A. Ryan, K. and Tag, A. Department of Biology, Texas A&M University.

DENATURATION AND PROTEIN FOLDING

Each protein has its own unique sequence and shape that chemical interactions hold together. If the protein is subject to changes in temperature, pH, or exposure to chemicals, the protein structure may change, losing its shape without losing its primary sequence in what scientists call denaturation. Denaturation is often reversible because the polypeptide's primary structure is conserved in the process if the denaturing agent is removed, allowing the protein to resume its function. Sometimes denaturation is irreversible, leading to loss of function. One example of irreversible protein denaturation is frying an egg. The albumin protein in the liquid egg white denatures when placed in a hot pan. Not all proteins denature at high temperatures. For instance, bacteria that survive in hot springs have proteins that function at temperatures close to boiling. The stomach is also very acidic, has a low pH, and denatures proteins as part of the digestion process; however, the stomach's digestive enzymes retain their activity under these conditions.

Protein folding is critical to its function. Scientists originally thought that the proteins themselves were responsible for the folding process. Only recently researchers discovered that often they receive assistance in the folding process from protein helpers, or chaperones (or chaperonins) that associate with the target protein during the folding process. They act by preventing polypeptide aggregation that comprise the complete protein structure, and they disassociate from the protein once the target protein is folded.

LINK TO LEARNING

LINK TO LEARNING

For an additional perspective on proteins, view this animation called “Biomolecules: The Proteins.”

This page titled 14.3: Primary Structure- Peptides is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

14.4: SECONDARY, TERTIARY, AND QUATERNARY STRUCTURE OF PROTEINS

LEARNING OBJECTIVES

By the end of this section, you will be able to do the following:

- Describe the functions proteins perform in the cell and in tissues
- Discuss the relationship between amino acids and proteins
- Explain the four levels of protein organization
- Describe the ways in which protein shape and function are linked

Proteins are one of the most abundant organic molecules in living systems and have the most diverse range of functions of all macromolecules. Proteins may be structural, regulatory, contractile, or protective. They may serve in transport, storage, or membranes; or they may be toxins or enzymes. Each cell in a living system may contain thousands of proteins, each with a unique function. Their structures, like their functions, vary greatly. They are all, however, amino acid polymers arranged in a linear sequence.

TYPES AND FUNCTIONS OF PROTEINS

Enzymes, which living cells produce, are catalysts in biochemical reactions (like digestion) and are usually complex or conjugated proteins. Each enzyme is specific for the substrate (a reactant that binds to an enzyme) upon which it acts. The enzyme may help in breakdown, rearrangement, or synthesis reactions. We call enzymes that break down their substrates catabolic enzymes. Those that build more complex molecules from their substrates are anabolic enzymes, and enzymes that affect the rate of reaction are catalytic enzymes. Note that all enzymes increase the reaction rate and, therefore, are organic catalysts. An example of an enzyme is salivary amylase, which hydrolyzes its substrate amylose, a component of starch.

Hormones are chemical-signaling molecules, usually small proteins or steroids, secreted by endocrine cells that act to control or regulate specific physiological processes, including growth, development, metabolism, and reproduction. For example, insulin is a protein hormone that helps regulate the blood glucose level. Table 3.1 lists the primary types and functions of proteins.

Protein Types and Functions

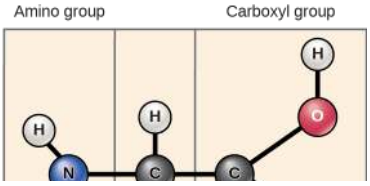
Type	Examples	Functions
Digestive Enzymes	Amylase, lipase, pepsin, trypsin	Help in food by catabolizing nutrients into monomeric units
Transport	Hemoglobin, albumin	Carry substances in the blood or lymph throughout the body
Structural	Actin, tubulin, keratin	Construct different structures, like the cytoskeleton
Hormones	Insulin, thyroxine	Coordinate different body systems' activity
Defense	Immunoglobulins	Protect the body from foreign pathogens
Contractile	Actin, myosin	Effect muscle contraction
Storage	Legume storage proteins, egg white (albumin)	Provide nourishment in early embryo development and the seedling

Table 3.1

Proteins have different shapes and molecular weights. Some proteins are globular in shape; whereas, others are fibrous in nature. For example, hemoglobin is a globular protein, but collagen, located in our skin, is a fibrous protein. Protein shape is critical to its function, and many different types of chemical bonds maintain this shape. Changes in temperature, pH, and exposure to chemicals may lead to permanent changes in the protein's shape, leading to loss of function, or denaturation. Different arrangements of the same 20 types of amino acids comprise all proteins. Two rare new amino acids were discovered recently (selenocystein and pirrolysine), and additional new discoveries may be added to the list.

AMINO ACIDS

Amino acids are the monomers that comprise proteins. Each amino acid has the same fundamental structure, which consists of a central carbon atom, or the alpha (α) carbon, bonded to an amino group (NH_2), a carboxyl group (COOH), and to a hydrogen atom. Every amino acid also has another atom or group of atoms bonded to the central atom known as the R group (Figure 3.22).



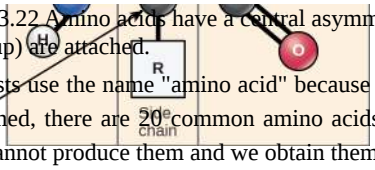


Figure 3.22 Amino acids have a central asymmetric carbon to which an amino group, a carboxyl group, a hydrogen atom, and a side chain (R group) are attached.

Scientists use the name "amino acid" because these acids contain both amino group and carboxyl-acid-group in their basic structure. As we mentioned, there are 20 common amino acids present in proteins. Nine of these are essential amino acids in humans because the human body cannot produce them and we obtain them from our diet. For each amino acid, the R group (or side chain) is different (Figure 3.23).

VISUAL CONNECTION

VISUAL CONNECTION

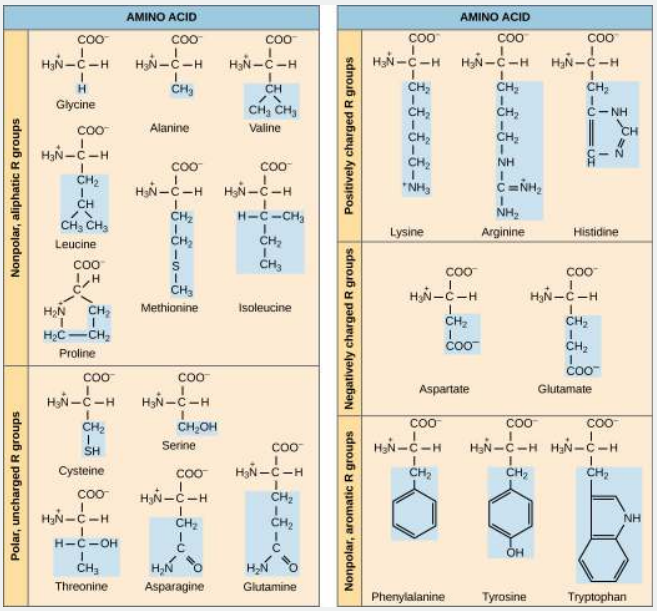


Figure 3.23 There are 20 common amino acids commonly found in proteins, each with a different R group (variant group) that determines its chemical nature.

Which categories of amino acid would you expect to find on a soluble protein's surface and which would you expect to find in the interior? What distribution of amino acids would you expect to find in a protein embedded in a lipid bilayer?

The chemical nature of the side chain determines the amino acid's nature (that is, whether it is acidic, basic, polar, or nonpolar). For example, the amino acid glycine has a hydrogen atom as the R group. Amino acids such as valine, methionine, and alanine are nonpolar or hydrophobic in nature, while amino acids such as serine, threonine, and cysteine are polar and have hydrophilic side chains. The side chains of lysine and arginine are positively charged, and therefore these amino acids are also basic amino acids. Proline has an R group that is linked to the amino group, forming a ring-like structure. Proline is an exception to the amino acid's standard structure since its amino group is not separate from the side chain (Figure 3.23).

A single upper case letter or a three-letter abbreviation represents amino acids. For example, the letter V or the three-letter symbol val represent valine. Just as some fatty acids are essential to a diet, some amino acids also are necessary. These essential amino acids in humans include isoleucine, leucine, and cysteine. Essential amino acids refer to those necessary to build proteins in the body, but not those that the body produces. Which amino acids are essential varies from organism to organism.

The sequence and the number of amino acids ultimately determine the protein's shape, size, and function. A covalent bond, or peptide bond, attaches to each amino acid, which a dehydration reaction forms. One amino acid's carboxyl group and the incoming amino acid's amino group combine, releasing a water molecule. The resulting bond is the peptide bond (Figure 3.24).

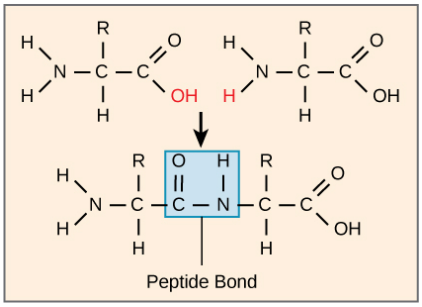


Figure 3.24 Peptide bond formation is a dehydration synthesis reaction. The carboxyl group of one amino acid is linked to the incoming amino acid's amino group. In the process, it releases a water molecule.

The products that such linkages form are peptides. As more amino acids join to this growing chain, the resulting chain is a polypeptide. Each polypeptide has a free amino group at one end. This end the N terminal, or the amino terminal, and the other end has a free carboxyl group, also the C or carboxyl terminal. While the terms polypeptide and protein are sometimes used interchangeably, a polypeptide is technically a polymer of amino acids, whereas the term protein is used for a polypeptide or polypeptides that have combined together, often have bound non-peptide prosthetic groups, have a distinct shape, and have a unique function. After protein synthesis (translation), most proteins are modified. These are known as post-translational modifications. They may undergo cleavage, phosphorylation, or may require adding other chemical groups. Only after these modifications is the protein completely functional.

LINK TO LEARNING

LINK TO LEARNING

Click through the steps of protein synthesis in this interactive tutorial.

EVOLUTION CONNECTION

EVOLUTION CONNECTION

The Evolutionary Significance of Cytochrome c

Cytochrome c is an important component of the electron transport chain, a part of cellular respiration, and it is normally located in the cellular organelle, the mitochondrion. This protein has a heme prosthetic group, and the heme's central ion alternately reduces and oxidizes during electron transfer. Because this essential protein's role in producing cellular energy is crucial, it has changed very little over millions of years. Protein sequencing has shown that there is a considerable amount of cytochrome c amino acid sequence homology among different species. In other words, we can assess evolutionary kinship by measuring the similarities or differences among various species' DNA or protein sequences.

Scientists have determined that human cytochrome c contains 104 amino acids. For each cytochrome c molecule from different organisms that scientists have sequenced to date, 37 of these amino acids appear in the same position in all cytochrome c samples. This indicates that there may have been a common ancestor. On comparing the human and chimpanzee protein sequences, scientists did not find a sequence difference. When researchers compared human and rhesus monkey sequences, the single difference was in one amino acid. In another comparison, human to yeast sequencing shows a difference in the 44th position.

PROTEIN STRUCTURE

As we discussed earlier, a protein's shape is critical to its function. For example, an enzyme can bind to a specific substrate at an active site. If this active site is altered because of local changes or changes in overall protein structure, the enzyme may be unable to bind to the substrate. To understand how the protein gets its final shape or conformation, we need to understand the four levels of protein structure: primary, secondary, tertiary, and quaternary.

PRIMARY STRUCTURE

Amino acids' unique sequence in a polypeptide chain is its primary structure. For example, the pancreatic hormone insulin has two polypeptide chains, A and B, and they are linked together by disulfide bonds. The N terminal amino acid of the A chain is glycine; whereas, the C terminal amino acid is asparagine (Figure 3.25). The amino acid sequences in the A and B chains are unique to insulin.

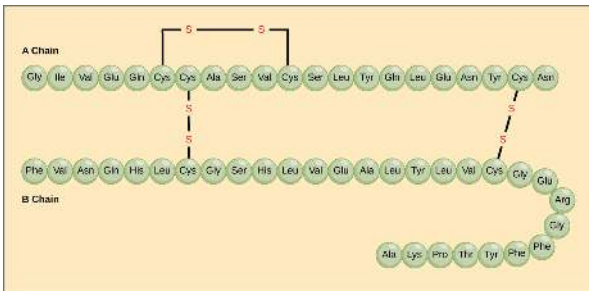


Figure 3.25 Bovine serum insulin is a protein hormone comprised of two peptide chains, A (21 amino acids long) and B (30 amino acids long). In each chain, three-letter abbreviations that represent the amino acids' names in the order they are present indicate primary structure. The amino acid cysteine (cys) has a sulfhydryl (SH) group as a side chain. Two sulfhydryl groups can react in the presence of oxygen to form a disulfide (S-S) bond. Two disulfide bonds connect the A and B chains together, and a third helps the A chain fold into the correct shape. Note that all disulfide bonds are the same length, but we have drawn them different sizes for clarity.

The gene encoding the protein ultimately determines the unique sequence for every protein. A change in nucleotide sequence of the gene's coding region may lead to adding a different amino acid to the growing polypeptide chain, causing a change in protein structure and function. In sickle cell anemia, the hemoglobin β chain (a small portion of which we show in Figure 3.26) has a single amino acid substitution, causing a change in protein structure and function. Specifically, valine in the β chain substitutes the amino acid glutamic. What is most remarkable to consider is that a hemoglobin molecule is comprised of two alpha and two beta chains that each consist of about 150 amino acids. The molecule, therefore, has about 600 amino acids. The structural difference between a normal hemoglobin molecule and a sickle cell molecule—which dramatically decreases life expectancy—is a single amino acid of the 600. What is even more remarkable is that three nucleotides each encode those 600 amino acids, and a single base change (point mutation), 1 in 1800 bases causes the mutation.

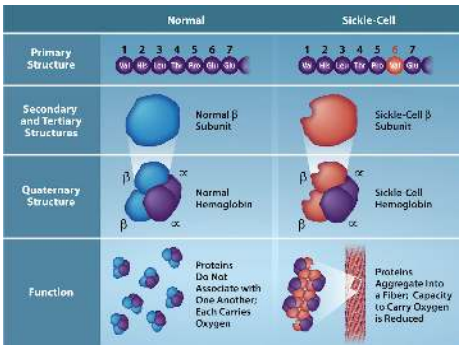


Figure 3.26 Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). .his 3.4 • Proteins 81 The beta (β)- chain of hemoglobin is 147 amino acids in length, yet a single amino acid substitution in the primary sequence leads changes in secondary, tertiary and quaternary structures and sickle cell anemia. In normal hemoglobin, the amino acid at position six is glutamate. In sickle cell hemoglobin glutamate is replaced by valine. Credit: Rao, A., Tag, A. Ryan, K. and Fletcher, S. Department of Biology, Texas A&M University.

Because of this change of one amino acid in the chain, hemoglobin molecules form long fibers that distort the biconcave, or disc-shaped, red blood cells and causes them to assume a crescent or "sickle" shape, which clogs blood vessels (Figure 3.27). This can lead to myriad serious health problems such as breathlessness, dizziness, headaches, and abdominal pain for those affected by this disease. William Warrick Cardozo showed that sickle-cell anemia is an inherited disorder, meaning that the difference in the specific gene's encoding region is passed down from parents to children. As you will learn in the genetics unit, the inheritance of such traits is determined by a combination of genes from both parents, and these very small differences can have significant impacts on organisms.

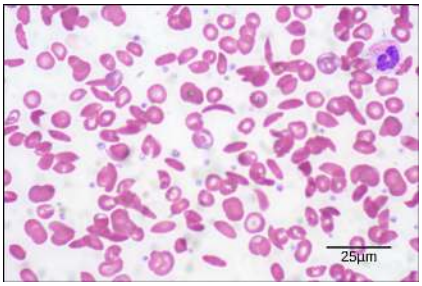


Figure 3.27 In this blood smear, visualized at 535x magnification using bright field microscopy, sickle cells are crescent shaped, while normal cells are disc-shaped. (credit: modification of work by Ed Uthman; scale-bar data from Matt Russell)

SECONDARY STRUCTURE

The local folding of the polypeptide in some regions gives rise to the secondary structure of the protein. The most common are the α-helix and β-pleated sheet structures (Figure 3.28). Both structures are held in shape by hydrogen bonds. The hydrogen bonds form between the oxygen atom in the carbonyl group in one amino acid and another amino acid that is four amino acids farther along the chain.

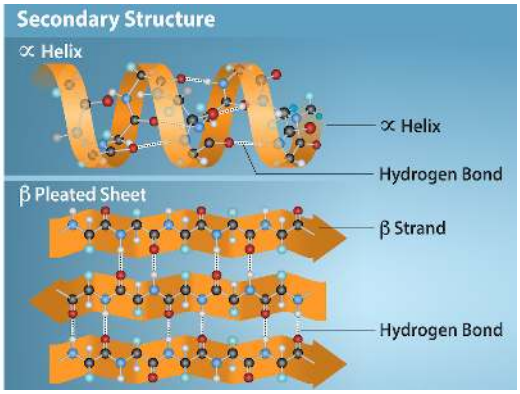


Figure 3.28 The α-helix and β-pleated sheet are secondary protein structures formed when hydrogen bonds form between the carbonyl oxygen and the amino hydrogen in the peptide backbone. Certain amino acids have a propensity to form an α-helix while others favor β-pleated sheet formation. Black = carbon, White = hydrogen, Blue = nitrogen, and Red = oxygen. Credit: Rao, A., Ryan, K. Fletcher, S. and Tag, A. Department of Biology, Texas A&M University.

Every helical turn in an alpha helix has 3.6 amino acid residues. The polypeptide's R groups (the variant groups) protrude out from the α-helix chain. In the β-pleated sheet, hydrogen bonding between atoms on the polypeptide chain's backbone form the "pleats". The R groups are attached to the carbons and extend above and below the pleat's folds. The pleated segments align parallel or antiparallel to each other, and hydrogen bonds form between the partially positive hydrogen atom in the amino group and the partially negative oxygen atom in the peptide backbone's carbonyl group. The α-helix and β-pleated sheet structures are in most globular and fibrous proteins and they play an important structural role.

TERTIARY STRUCTURE

The polypeptide's unique three-dimensional structure is its tertiary structure (Figure 3.29). This structure is in part due to chemical interactions at work on the polypeptide chain. Primarily, the interactions among R groups create the protein's complex three-dimensional tertiary structure. The nature of the R groups in the amino acids involved can counteract forming the hydrogen bonds we described for standard secondary structures. For example, R groups with like charges repel each other and those with unlike charges are attracted to each other (ionic bonds). When protein folding takes place, the nonpolar amino acids' hydrophobic R groups lie in the protein's interior; whereas, the hydrophilic R groups lie on the outside. Scientists also call the former interaction types hydrophobic interactions. Interaction between cysteine side chains forms disulfide linkages in the presence of oxygen, the only covalent bond that forms during protein folding.

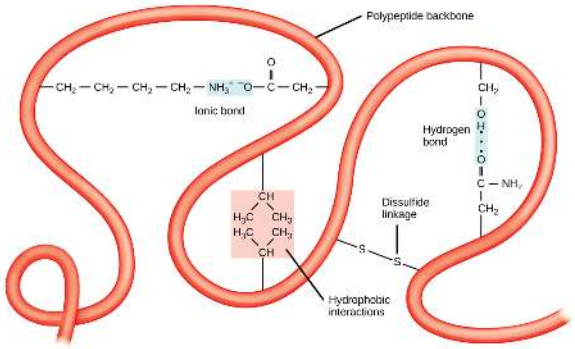


Figure 3.29 A variety of chemical interactions determine the proteins' tertiary structure. These include hydrophobic interactions, ionic bonding, hydrogen bonding, and disulfide linkages.

All of these interactions, weak and strong, determine the protein's final three-dimensional shape. When a protein loses its three-dimensional shape, it may no longer be functional.

QUATERNARY STRUCTURE

In nature, some proteins form from several polypeptides, or subunits, and the interaction of these subunits forms the quaternary structure. Weak interactions between the subunits help to stabilize the overall structure. For example, insulin (a globular protein) has a combination of hydrogen and disulfide bonds that cause it to mostly clump into a ball shape. Insulin starts out as a single polypeptide and loses some internal sequences in the presence of post-translational modification after forming the disulfide linkages that hold the remaining chains together. Silk (a fibrous protein), however, has a β-pleated sheet structure that is the result of hydrogen bonding between different chains.

Figure 3.30 illustrates the four levels of protein structure (primary, secondary, tertiary, and quaternary).

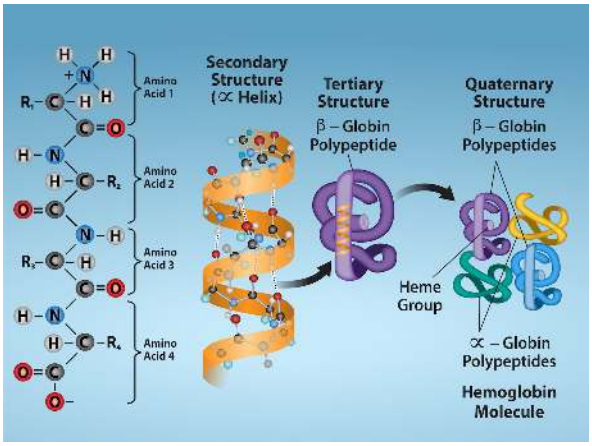


Figure 3.30 Observe the four levels of protein structure in these illustrations. Credit: Rao, A. Ryan, K. and Tag, A. Department of Biology, Texas A&M University.

DENATURATION AND PROTEIN FOLDING

Each protein has its own unique sequence and shape that chemical interactions hold together. If the protein is subject to changes in temperature, pH, or exposure to chemicals, the protein structure may change, losing its shape without losing its primary sequence in what scientists call denaturation. Denaturation is often reversible because the polypeptide's primary structure is conserved in the process if the denaturing agent is removed, allowing the protein to resume its function. Sometimes denaturation is irreversible, leading to loss of function. One example of irreversible protein denaturation is frying an egg. The albumin protein in the liquid egg white denatures when placed in a hot pan. Not all proteins denature at high temperatures. For instance, bacteria that survive in hot springs have proteins that function at temperatures close to boiling. The stomach is also very acidic, has a low pH, and denatures proteins as part of the digestion process; however, the stomach's digestive enzymes retain their activity under these conditions.

Protein folding is critical to its function. Scientists originally thought that the proteins themselves were responsible for the folding process. Only recently researchers discovered that often they receive assistance in the folding process from protein helpers, or chaperones (or chaperonins) that associate with the target protein during the folding process. They act by preventing polypeptide aggregation that comprise the complete protein structure, and they disassociate from the protein once the target protein is folded.

LINK TO LEARNING

LINK TO LEARNING

For an additional perspective on proteins, view this animation called “Biomolecules: The Proteins.”

This page titled 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

14.5: Case Study- Synergy in Science and Care - Protein Structures Illuminating Metabolic Disorder Management

Introduction: The nuanced study of protein structures is a multidisciplinary endeavor critical to understanding and managing metabolic disorders. In a collaborative clinical research setting, the collective expertise of biochemists, geneticists, computational biologists, and nursing professionals is essential for translating molecular insights into meaningful patient care. This case study examines how such an integrated team approach can elucidate the role of protein structures in metabolic diseases.

Scenario: At the Genotech Research Institute, Dr. Emily Wong, a biochemist, spearheads a diverse research team with expertise spanning several scientific and clinical disciplines. The team includes a geneticist who provides insights into the genetic underpinnings of protein structures, a computational biologist who models these structures and predicts their function, and a nurse who brings a practical understanding of patient care and disease manifestation. Together, they work on understanding the enzyme dysfunction in a pediatric patient named Lucas, who is grappling with a metabolic disorder.

Multifaceted Investigation of Proteins: The team collectively examines the enzyme's primary structure, with the geneticist pinpointing the genetic mutations affecting amino acid sequences. The computational biologist models the secondary and tertiary structures, predicting how mutations might alter the enzyme's shape and function. The biochemist, Dr. Wong, provides the biochemical framework for understanding these structures, while the nurse, equipped with firsthand knowledge of Lucas's daily health struggles, contextualizes the scientific data within the patient's experience.

Case Study Questions:

1. **Describe the primary, secondary, and tertiary structure of proteins.**
2. **How does protein structure influence disease development?**

Hands-On Classroom Activities:

1. **Protein Folding Simulation: I**n the "Protein Folding Simulation," students will utilize origami as a hands-on model to simulate the process of protein folding, and they will subsequently discuss the potential consequences that misfolded proteins can have on cellular function and disease.
2. **Enzyme Activity Lab:** The "Enzyme Activity Lab" provides students with an opportunity to study the activity of enzymes by experimenting with various substrates and temperatures, thereby allowing them to observe firsthand how these factors influence enzyme behavior and relate to the enzyme's protein structure.

Conclusion: In this interdisciplinary framework, each team member's unique perspective is vital to unraveling the complex relationship between protein structure and metabolic disorders. The biochemist's chemical expertise, the geneticist's understanding of hereditary influence, the computational biologist's structural predictions, and the nurse's patient-centered approach collectively provide a comprehensive understanding of Lucas's condition. This case study demonstrates the power of a multidisciplinary team in advancing both scientific understanding and patient care in the context of metabolic health.

14.5: Case Study- Synergy in Science and Care - Protein Structures Illuminating Metabolic Disorder Management is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

14.6: 3D Printing Activity- Protein-Ligand Binding

14.6: 3D Printing Activity- Protein-Ligand Binding is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

14.E: Exercises

Multiple Choice

1. Which of the following is a nonpolar (hydrophobic) amino acid?

    a) tyrosine

    b) serine

    c) valine

    d) lysine

2. Which of the following elements is not found in amino acids?

    a) hydrogen

    b) phosphorus

    c) oxygen

    d) nitrogen

3. Which one of the following statements about amino acids is true?

    a) Twenty-four different amino acids are commonly found in proteins

    b) All amino acids contain a carboxylic acid group

    c) Amino acids with hydrophobic side chains are insoluble in water

    d) Amino acids are linked via a “backbone” of sugar-phosphate bonds

4. Which of the following statements is **not** true of the amino acids?

    a) Some amino acids are obtained only from foods we eat.

    b) The R group of amino acids differs from one amino acid to another.

    c) Amino acids have an N-terminus, C-terminus, and R groups.

    d) All amino acids exist in two stereoisomeric forms.

5. The chemical nature of each amino acid is determined by which of the following groups?

    a) amino

    b) carboxyl

    c) hydroxyl

    d) R group (side chain)

6. An amino acid is made up of:

    a) alpha carbon linked to hydrogen, hydroxyl group, amino group, and a side chain

    b) alpha carbon linked to hydrogen, amino group and carboxylic acid group

    c) alpha carbon linked to hydrogen, amino group, carboxylic acid group, and a side chain

    d) alpha carbon linked to hydrogen, hydroxyl group, amino group, and a carboxylic acid group

7. Which group of three amino acid side chains can form hydrogen bonds with one another?

    a) serine, aspartic acid, threonine

    b) phenylalanine, isoleucine, glycine

    c) aspartic acid, valine, threonine

d) alanine, tryptophan, histidine

8. Which amino acids would you most expect to find inside a protein's 3-D structure, away from water?

a) serine, glutamic acid, tyrosine

b) phenylalanine, isoleucine, glycine

c) aspartic acid, valine, threonine

d) alanine, tryptophan, histidine

9. Can glycine form hydrogen bonds with other amino acids?

a) Yes, because it forms random coils between strands of beta sheets.

b) No, because it is nonpolar.

c) Yes, because it is contains an alpha carbon.

d) Yes, because it contains a C=O bond and an N-H bond.

10. What is the side chain (R group) on glycine?

a) -C=O

b) -N-H

c) $-CH_2-CH_3$

d) -H

11. The primary structure of a protein

a) is the order of amino acids from one end of the protein to another.

b) is important both genetically and structurally.

c) is the linear sequence of amino acids that are linked together by peptide bonds.

d) all of the above

12. Do all polypeptides have tertiary structure?

a) Yes, because they all have secondary structures that are arranged in 3D space.

b) No, because only proteins have tertiary structure.

c) Yes, because they fold into three types of shapes.

d) No, because polypeptides are smaller parts of protein complexes.

13. Hydrogen bonding is most important in stabilizing the _____ structure of many proteins.

a) primary

b) secondary

c) tertiary

d) quaternary

14. Phosphodiester bonds and peptide bonds share an important feature. What is it?

a) Both are created by dehydration reactions

b) Both are found in proteins

c) Both are used to store high-energy electrons

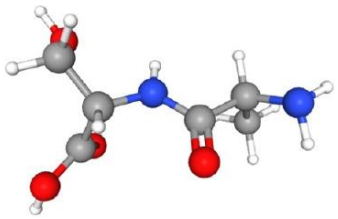
d) Both are formed by the same enzymes

Warm-Up Questions

1-6. Decide which amino acids best fit the following descriptions:

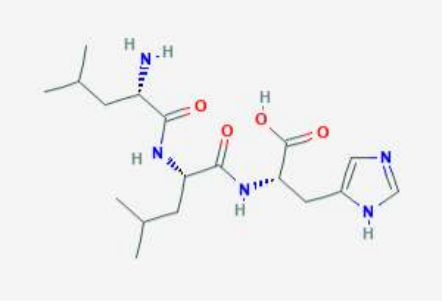
1. _____ has a nonpolar sidechain and interacts with other aromatic rings.
2. _____ is small, and it does not contain sulfur. It can form hydrogen bonds.
3. _____ The lone electron pair at one of the ring nitrogens makes it important in stabilizing the iron atoms in myoglobin.
4. _____ has an extended basic sidechain.
5. _____ is a bulky, hydrophobic amino acid with a double ring structure
6. _____ is the first amino acid in a primary sequence

7. The image below shows a ball-and-stick model of the dipeptide made of alanine and serine. You can access an interactive model of the molecule here. Indicate the location of the amino-terminus, the carboxyl-terminus, the peptide bond and the R groups on alanine and serine.



https://pubchem.ncbi.nlm.nih.gov/compound/Ala-Ser

8. The image below shows a 2-D structural model of the tripeptide Leu-Leu-His. Indicate the location of the amino-terminus, the carboxyl-terminus, the peptide bond and the three R groups.



https://pubchem.ncbi.nlm.nih.gov/compound/49864737

Intermediate Questions

1. Explain the chemical features that make proline distinct from other amino acids.

2. Explain why glycine is classified as a non-polar amino acid in proteins.

3. Draw a dipeptide consisting of a polar amino acid at the amino terminus and a non-polar amino acid at the carboxyl terminus.

4. Draw the dipeptide consisting of the amino acid with the shortest R group (other than glycine) at the amino terminus and the amino acid with the largest R group at the carboxyl terminus.

5. What is the net charge on a peptide with the sequence N-Met-Ser-Arg-Gly-Gly-Glu-Ala-Val-Lys-C at physiological pH?

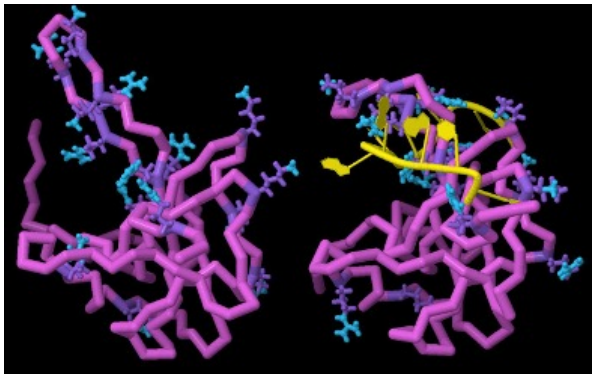
6. What is the net charge on a peptide with the sequence N-Ser-Gly-Tyr-Ile-His-Arg-C at physiological pH?

7. This image shows a “ribbon” structure of the protein phospholipase A2, an enzyme that breaks apart phospholipids. You can access an interactive 3D model of the protein here. Comment on the overall structure of the protein and indicate examples of secondary structure.



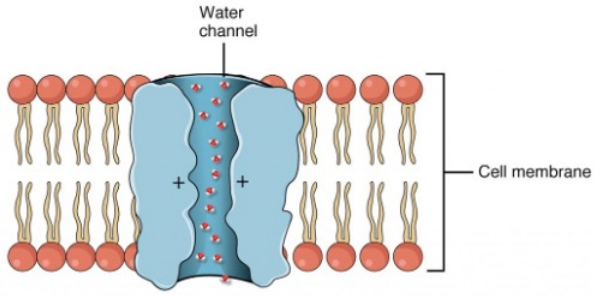
https://doi.org/10.2210/pdb1CJY/pdb

8. The image below shows a portion of the protein nucleocapsid, which is encoded by the genome for SARS-CoV-2 (the virus that causes COVID-19). Nucleocapsid binds to viral RNA and packages it into new virus particles inside infected host cells. The image shows the protein alone on the left side, and protein bound to RNA on the right side. RNA is in yellow, the peptide backbone is in magenta, and select amino acid side chains are in purple and turquoise. Identify the amino acids and explain why their structure helps with RNA binding.



Challenge Questions

1. The image below depicts a cross-section of a cell membrane in which a channel protein called aquaporin is embedded. Describe the structural features of the protein. What amino acids are likely to be on the protein exterior, or inside the water channel?



https://ecampusontario.pressbooks.pub/app/uploads/sites/159/2018/07/2625_Aquaporin_Water_Channel-1024x515.jpg

2. Describe the types of bonds/interactions that hold together or stabilize the primary, secondary, tertiary, and quaternary structures of proteins.

Health-Related Questions

1. Changes in temperature and pH, such as found in febrile state or during digestion in the gut, can inactivate proteins by causing them to unfold or misfold. Explain the chemical basis of protein unfolding.

2. Albumin is the most abundant protein in blood serum (approximately 4.0 g/dl) and is an indicator of overall health. Albumin plays an important role as a carrier of fatty acids in the bloodstream. It can also bind to drug molecules and facilitate their transport through the body. Follow the link below to view an interactive 3-D representation of human serum albumin with molecules of stearic acid incorporated into the structure. Use the toolbar at the top of the page to change the way protein and lipid components are displayed. Comment on the secondary and tertiary structure of the protein, the number of stearic acid molecules that are present, and their orientation in the overall structure. Given what you know about lipids, do you think that albumin binding is specific to stearic acid?

https://www.ncbi.nlm.nih.gov/Structure/icn3d/full.html?mmdbid=1E7I&bu=1

14.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

15: Molecular Genetics

15.1: DNA Structure

15.2: Case Study- Decoding Disease - The Role of DNA Structure in Genetic Disorders

15.E: Exercises

15: Molecular Genetics is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

15.1: DNA Structure

Learning Objectives

- Describe the biochemical structure of deoxyribonucleotides
- Identify the base pairs used in the synthesis of deoxyribonucleotides
- Explain why the double helix of DNA is described as antiparallel

In Microbial Metabolism, we discussed three classes of macromolecules: proteins, lipids, and carbohydrates. In this chapter, we will discuss a fourth class of macromolecules: nucleic acids. Like other macromolecules, nucleic acids are composed of monomers, called nucleotides, which are polymerized to form large strands. Each nucleic acid strand contains certain nucleotides that appear in a certain order within the strand, called its base sequence. The base sequence of deoxyribonucleic acid (DNA) is responsible for carrying and retaining the hereditary information in a cell. In Mechanisms of Microbial Genetics, we will discuss in detail the ways in which DNA uses its own base sequence to direct its own synthesis, as well as the synthesis of RNA and proteins, which, in turn, gives rise to products with diverse structure and function. In this section, we will discuss the basic structure and function of DNA.

DNA Nucleotides

The building blocks of nucleic acids are nucleotides. Nucleotides that compose DNA are called deoxyribonucleotides. The three components of a deoxyribonucleotide are a five-carbon sugar called deoxyribose, a phosphate group, and a nitrogenous base, a nitrogen-containing ring structure that is responsible for complementary base pairing between nucleic acid strands (Figure 15.1.1). The carbon atoms of the five-carbon deoxyribose are numbered 1′, 2′, 3′, 4′, and 5′ (1′ is read as “one prime”). A nucleoside comprises the five-carbon sugar and nitrogenous base.

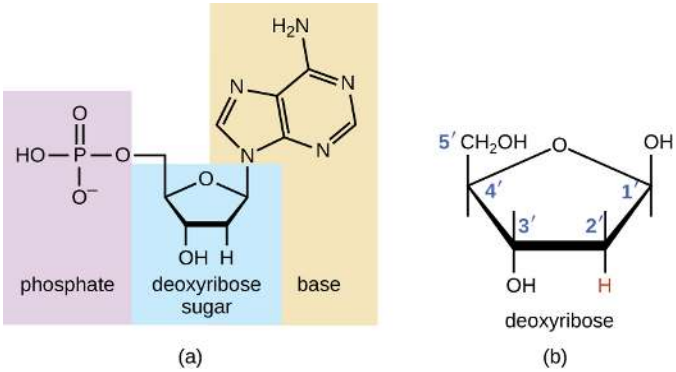


Figure 15.1.1: (a) Each deoxyribonucleotide is made up of a sugar called deoxyribose, a phosphate group, and a nitrogenous base—in this case, adenine. (b) The five carbons within deoxyribose are designated as 1′, 2′, 3′, 4′, and 5′.

The deoxyribonucleotide is named according to the nitrogenous bases (Figure 15.1.2). The nitrogenous bases adenine (A) and guanine (G) are the purines; they have a double-ring structure with a six-carbon ring fused to a five-carbon ring. The pyrimidines, cytosine (C) and thymine (T), are smaller nitrogenous bases that have only a six-carbon ring structure.

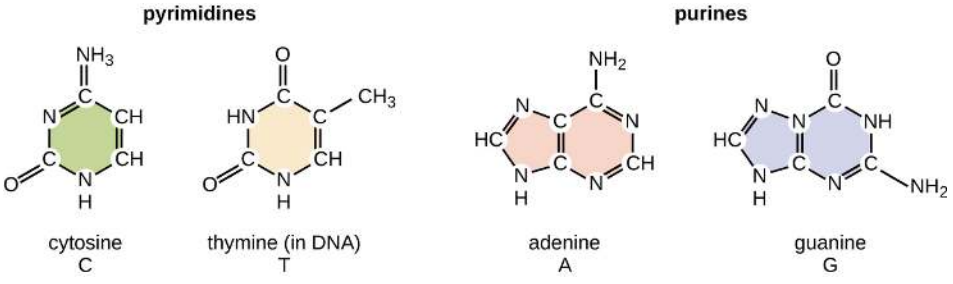


Figure 15.1.2: Nitrogenous bases within DNA are categorized into the two-ringed purines adenine and guanine and the single-ringed pyrimidines cytosine and thymine. Thymine is unique to DNA.

Individual nucleoside triphosphates combine with each other by covalent bonds known as 5′-3′ phosphodiester bonds, or linkages whereby the phosphate group attached to the 5′ carbon of the sugar of one nucleotide bonds to the hydroxyl group of the 3′ carbon

of the sugar of the next nucleotide. Phosphodiester bonding between nucleotides forms the sugar-phosphate backbone, the alternating sugar-phosphate structure composing the framework of a nucleic acid strand (Figure **15.1.3**). During the polymerization process, deoxynucleotide triphosphates (dNTP) are used. To construct the sugar-phosphate backbone, the two terminal phosphates are released from the dNTP as a pyrophosphate. The resulting strand of nucleic acid has a free phosphate group at the 5′ carbon end and a free hydroxyl group at the 3′ carbon end. The two unused phosphate groups from the nucleotide triphosphate are released as pyrophosphate during phosphodiester bond formation. Pyrophosphate is subsequently hydrolyzed, releasing the energy used to drive nucleotide polymerization.

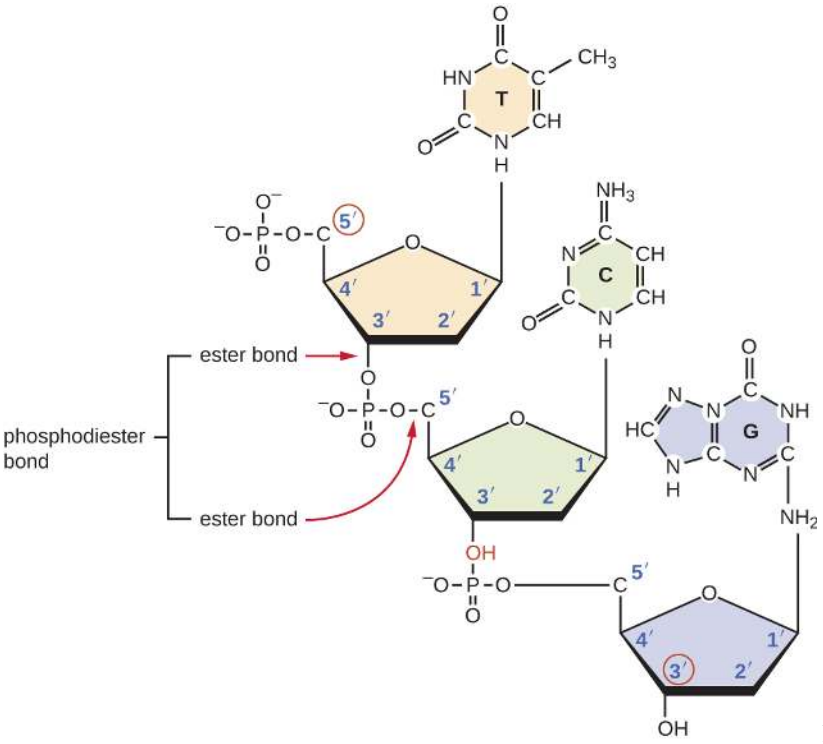


Figure **15.1.3**: Phosphodiester bonds form between the phosphate group attached to the 5′ carbon of one nucleotide and the hydroxyl group of the 3′ carbon in the next nucleotide, bringing about polymerization of nucleotides in to nucleic acid strands. Note the 5′ and 3′ ends of this nucleic acid strand.

? Exercise 15.1.1

What is meant by the 5′ and 3′ ends of a nucleic acid strand?

Discovering the Double Helix

By the early 1950s, considerable evidence had accumulated indicating that DNA was the genetic material of cells, and now the race was on to discover its three-dimensional structure. Around this time, Austrian biochemist Erwin Chargaff[1](1905–2002) examined the content of DNA in different species and discovered that adenine, thymine, guanine, and cytosine were not found in equal quantities, and that it varied from species to species, but not between individuals of the same species. He found that the amount of adenine was very close to equaling the amount of thymine, and the amount of cytosine was very close to equaling the amount of guanine, or A = T and G = C. These relationships are also known as Chargaff's rules.

Other scientists were also actively exploring this field during the mid-20th century. In 1952, American scientist Linus Pauling (1901–1994) was the world's leading structural chemist and odds-on favorite to solve the structure of DNA. Pauling had earlier discovered the structure of protein α helices, using X-ray diffraction, and, based upon X-ray diffraction images of DNA made in his laboratory, he proposed a triple-stranded model of DNA.[2] At the same time, British researchers Rosalind Franklin (1920–1958) and her graduate student R.G. Gosling were also using X-ray diffraction to understand the structure of DNA (Figure **15.1.4**). It was Franklin's scientific expertise that resulted in the production of more well-defined X-ray diffraction images of DNA that would clearly show the overall double-helix structure of DNA.

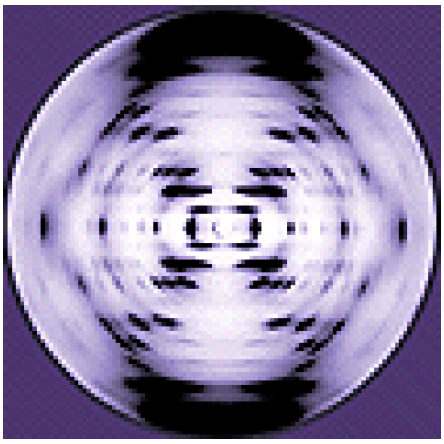


Figure **15.1.4**: The X-ray diffraction pattern of DNA shows its helical nature. (credit: National Institutes of Health)

James Watson (1928–), an American scientist, and Francis Crick (1916–2004), a British scientist, were working together in the 1950s to discover DNA's structure. They used Chargaff's rules and Franklin and Wilkins' X-ray diffractionimages of DNA fibers to piece together the purine-pyrimidine pairing of the double helical DNA molecule (Figure **15.1.5**). In April 1953, Watson and Crick published their model of the DNA double helix in *Nature*.[3] The same issue additionally included papers by Wilkins and colleagues,[4] as well as by Franklin and Gosling,[5] each describing different aspects of the molecular structure of DNA. In 1962, James Watson, Francis Crick, and Maurice Wilkins were awarded the Nobel Prize in Physiology and Medicine. Unfortunately, by then Franklin had died, and Nobel prizes at the time were not awarded posthumously. Work continued, however, on learning about the structure of DNA. In 1973, Alexander Rich(1924–2015) and colleagues were able to analyze DNA crystals to confirm and further elucidate DNA structure.[6]



Figure **15.1.5**: In 1953, James Watson and Francis Crick built this model of the structure of DNA, shown here on display at the Science Museum in London.

? Exercise 15.1.2

Which scientists are given most of the credit for describing the molecular structure of DNA?

DNA Structure

Watson and Crick proposed that DNA is made up of two strands that are twisted around each other to form a right-handed helix. The two DNA strands are antiparallel, such that the 3′ end of one strand faces the 5′ end of the other (Figure **15.1.6**). The 3′ end of each strand has a free hydroxyl group, while the 5′ end of each strand has a free phosphate group. The sugar and phosphate of the polymerized nucleotides form the backbone of the structure, whereas the nitrogenous bases are stacked inside. These nitrogenous bases on the interior of the molecule interact with each other, base pairing.

Analysis of the diffraction patterns of DNA has determined that there are approximately 10 bases per turn in DNA. The asymmetrical spacing of the sugar-phosphate backbones generates major grooves (where the backbone is far apart) and minor grooves (where the backbone is close together) (Figure 15.1.6). These grooves are locations where proteins can bind to DNA. The binding of these proteins can alter the structure of DNA, regulate replication, or regulate transcription of DNA into RNA.

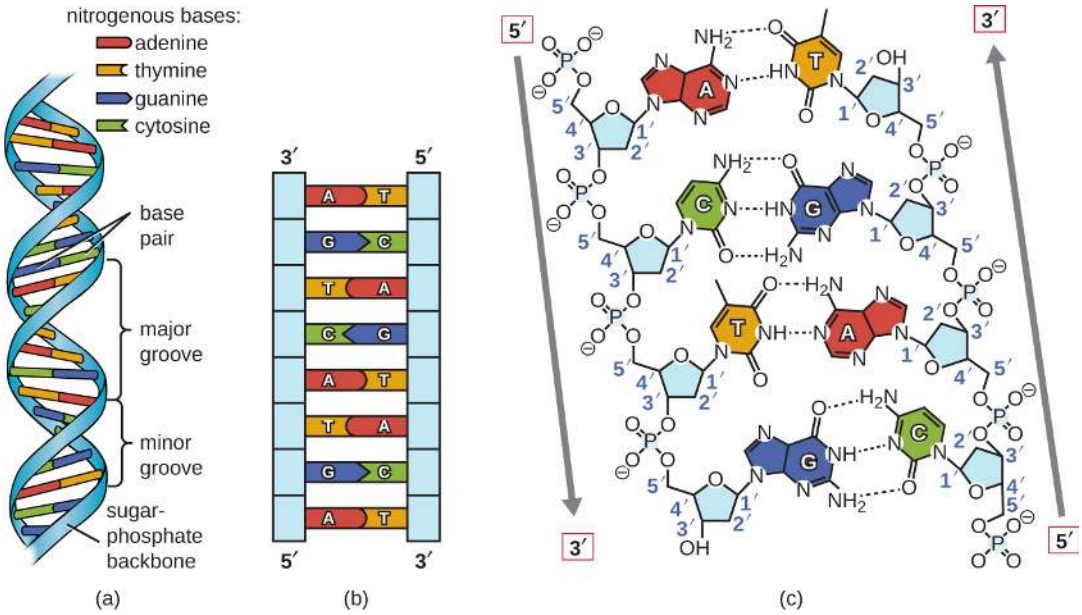


Figure 15.1.6: Watson and Crick proposed the double helix model for DNA. (a) The sugar-phosphate backbones are on the outside of the double helix and purines and pyrimidines form the "rungs" of the DNA helix ladder. (b) The two DNA strands are antiparallel to each other. (c) The direction of each strand is identified by numbering the carbons (1 through 5) in each sugar molecule. The 5′ end is the one where carbon #5 is not bound to another nucleotide; the 3′ end is the one where carbon #3 is not bound to another nucleotide.

Base pairing takes place between a purine and pyrimidine. In DNA, adenine (A) and thymine (T) are complementary base pairs, and cytosine (C) and guanine (G) are also complementary base pairs, explaining Chargaff's rules (Figure 15.1.7). The base pairs are stabilized by hydrogen bonds; adenine and thymine form two hydrogen bonds between them, whereas cytosine and guanine form three hydrogen bonds between them.

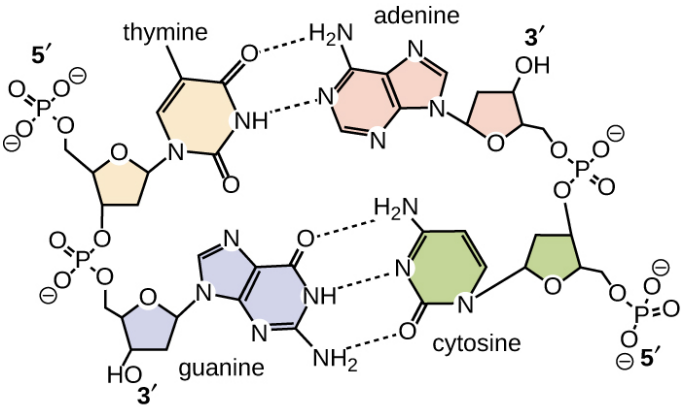


Figure 15.1.7: Hydrogen bonds form between complementary nitrogenous bases on the interior of DNA.

In the laboratory, exposing the two DNA strands of the double helix to high temperatures or to certain chemicals can break the hydrogen bonds between complementary bases, thus separating the strands into two separate single strands of DNA (single-stranded DNA [ssDNA]). This process is called DNA denaturation and is analogous to protein denaturation, as described in Proteins. The ssDNA strands can also be put back together as double-stranded DNA (dsDNA), through reannealing or renaturing by cooling or removing the chemical denaturants, allowing these hydrogen bonds to reform. The ability to artificially manipulate DNA in this way is the basis for several important techniques in biotechnology (Figure 15.1.8). Because of the additional hydrogen

bonding between the C = G base pair, DNA with a high GC content is more difficult to denature than DNA with a lower GC content.

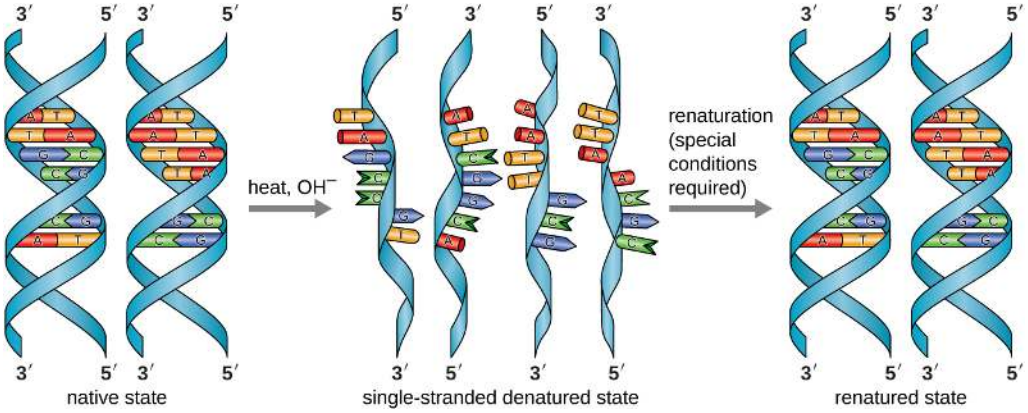


Figure 15.1.8: In the laboratory, the double helix can be denatured to single-stranded DNA through exposure to heat or chemicals, and then renatured through cooling or removal of chemical denaturants to allow the DNA strands to reanneal. (credit: modification of work by Hernández-Lemus E, Nicasio-Collazo LA, Castañeda-Priego R)

Link to Learning

View an animation on DNA structure from the DNA Learning Center to learn more.

Exercise 15.1.3

What are the two complementary base pairs of DNA and how are they bonded together?

DNA Function

DNA stores the information needed to build and control the cell. The transmission of this information from mother to daughter cells is called vertical gene transfer and it occurs through the process of DNA replication. DNA is replicated when a cell makes a duplicate copy of its DNA, then the cell divides, resulting in the correct distribution of one DNA copy to each resulting cell. DNA can also be enzymatically degraded and used as a source of nucleosides and nucleotides for the cell. Unlike other macromolecules, DNA does not serve a structural role in cells.

Exercise 15.1.4

How does DNA transmit genetic information to offspring?

Paving the Way for Women in Science and Health Professions

Historically, women have been underrepresented in the sciences and in medicine, and often their pioneering contributions have gone relatively unnoticed. For example, although Rosalind Franklin performed the X-ray diffraction studies demonstrating the double helical structure of DNA, it is Watson and Crick who became famous for this discovery, building on her data. There still remains great controversy over whether their acquisition of her data was appropriate and whether personality conflicts and gender bias contributed to the delayed recognition of her significant contributions. Similarly, Barbara McClintock did pioneering work in maize (corn) genetics from the 1930s through 1950s, discovering transposons (jumping genes), but she was not recognized until much later, receiving a Nobel Prize in Physiology or Medicine in 1983 (Figure 15.1.9).

Today, women still remain underrepresented in many fields of science and medicine. While more than half of the undergraduate degrees in science are awarded to women, only 46% of doctoral degrees in science are awarded to women. In academia, the number of women at each level of career advancement continues to decrease, with women holding less than one-third of the positions of Ph.D.-level scientists in tenure-track positions, and less than one-quarter of the full professorships at 4-year colleges and universities.[7] Even in the health professions, like nearly all other fields, women are often underrepresented in

many medical careers and earn significantly less than their male counterparts, as shown in a 2013 study published by the *Journal of the American Medical Association*.[8]

Why do such disparities continue to exist and how do we break these cycles? The situation is complex and likely results from the combination of various factors, including how society conditions the behaviors of girls from a young age and supports their interests, both professionally and personally. Some have suggested that women do not belong in the laboratory, including Nobel Prize winner Tim Hunt, whose 2015 public comments suggesting that women are too emotional for science[9] were met with widespread condemnation.

Perhaps girls should be supported more from a young age in the areas of science and math (Figure **15.1.9**). Science, technology, engineering, and mathematics (STEM) programs sponsored by the American Association of University Women (AAUW)[10] and National Aeronautics and Space Administration (NASA)[11] are excellent examples of programs that offer such support. Contributions by women in science should be made known more widely to the public, and marketing targeted to young girls should include more images of historically and professionally successful female scientists and medical professionals, encouraging all bright young minds, including girls and women, to pursue careers in science and medicine.



Figure **15.1.9**: (a) Barbara McClintock's work on maize genetics in the 1930s through 1950s resulted in the discovery of transposons, but its significance was not recognized at the time. (b) Efforts to appropriately mentor and to provide continued societal support for women in science and medicine may someday help alleviate some of the issues preventing gender equality at all levels in science and medicine. (credit a: modification of work by Smithsonian Institution; credit b: modification of work by Haynie SL, Hinkle AS, Jones NL, Martin CA, Olsiewski PJ, Roberts MF)

Clinical Focus: Part 2

Based upon his symptoms, Alex's physician suspects that he is suffering from a foodborne illness that he acquired during his travels. Possibilities include bacterial infection (e.g., enterotoxigenic *E. coli*, *Vibrio cholerae*, *Campylobacter jejuni*, *Salmonella*), viral infection (rotavirus or norovirus), or protozoan infection (*Giardia lamblia*, *Cryptosporidium parvum*, or *Entamoeba histolytica*).

His physician orders a stool sample to identify possible causative agents (e.g., bacteria, cysts) and to look for the presence of blood because certain types of infectious agents (like *C. jejuni*, *Salmonella*, and *E. histolytica*) are associated with the production of bloody stools.

Alex's stool sample showed neither blood nor cysts. Following analysis of his stool sample and based upon his recent travel history, the hospital physician suspected that Alex was suffering from traveler's diarrhea caused by enterotoxigenic *E. coli* (ETEC), the causative agent of most traveler's diarrhea. To verify the diagnosis and rule out other possibilities, Alex's physician ordered a diagnostic lab test of his stool sample to look for DNA sequences encoding specific virulence factors of ETEC. The physician instructed Alex to drink lots of fluids to replace what he was losing and discharged him from the hospital.

ETEC produces several plasmid-encoded virulence factors that make it pathogenic compared with typical *E. coli*. These include the secreted toxins heat-labile enterotoxin (LT) and heat-stabile enterotoxin (ST), as well as colonization factor (CF). Both LT and ST cause the excretion of chloride ions from intestinal cells to the intestinal lumen, causing a consequent loss of

water from intestinal cells, resulting in diarrhea. CF encodes a bacterial protein that aids in allowing the bacterium to adhere to the lining of the small intestine.

Exercise 15.1.5

Why did Alex's physician use genetic analysis instead of either isolation of bacteria from the stool sample or direct Gram stain of the stool sample alone?

Key Concepts and Summary

- **Nucleic acids** are composed of **nucleotides**, each of which contains a pentose sugar, a phosphate group, and a **nitrogenous base**. **Deoxyribonucleotides** within DNA contain **deoxyribose** as the pentose sugar.
- DNA contains the **pyrimidines cytosine** and **thymine**, and the **purines adenine** and **guanine**.
- **Nucleotides** are linked together by phosphodiester bonds between the 5′ phosphate group of one nucleotide and the 3′ hydroxyl group of another. A **nucleic acid strand** has a free phosphate group at the 5′ end and a free hydroxyl group at the 3′ end.
- Chargaff discovered that the amount of **adenine** is approximately equal to the amount of **thymine** in DNA, and that the amount of the **guanine** is approximately equal to **cytosine**. These relationships were later determined to be due to complementary base pairing.
- Watson and Crick, building on the work of Chargaff, Franklin and Gosling, and Wilkins, proposed the double helix model and base pairing for DNA structure.
- DNA is composed of two complementary strands oriented **antiparallel** to each other with the **phosphodiester backbones** on the exterior of the molecule. The nitrogenous bases of each strand face each other and complementary bases hydrogen bond to each other, stabilizing the double helix.
- Heat or chemicals can break the hydrogen bonds between complementary bases, denaturing DNA. Cooling or removing chemicals can lead to renaturation or reannealing of DNA by allowing hydrogen bonds to reform between complementary bases.
- DNA stores the instructions needed to build and control the cell. This information is transmitted from parent to offspring through **vertical gene transfer**.

Footnotes

1. 1 N. Kresge et al. "Chargaff's Rules: The Work of Erwin Chargaff." *Journal of Biological Chemistry* 280 (2005):e21.
2. 2 L. Pauling, "A Proposed Structure for the Nucleic Acids." *Proceedings of the National Academy of Science of the United States of America* 39 no. 2 (1953):84–97.
3. 3 J.D. Watson, F.H.C. Crick. "A Structure for Deoxyribose Nucleic Acid." *Nature* 171 no. 4356 (1953):737–738.
4. 4 M.H.F. Wilkins et al. "Molecular Structure of Deoxypentose Nucleic Acids." *Nature* 171 no. 4356 (1953):738–740.
5. 5 R. Franklin, R.G. Gosling. "Molecular Configuration in Sodium Thymonucleate." *Nature* 171 no. 4356 (1953):740–741.
6. 6 R.O. Day et al. "A Crystalline Fragment of the Double Helix: The Structure of the Dinucleoside Phosphate Guanylyl-3',5'-Cytidine." *Proceedings of the National Academy of Sciences of the United States of America* 70 no. 3 (1973):849–853.
7. 7 N.H. Wolfinger "For Female Scientists, There's No Good Time to Have Children." *The Atlantic* July 29, 2013. www.theatlantic.com/sexes/arc...ildren/278165/.
8. 8 S.A. Seabury et al. "Trends in the Earnings of Male and Female Health Care Professionals in the United States, 1987 to 2010." *Journal of the American Medical Association Internal Medicine* 173 no. 18 (2013):1748–1750.
9. 9 E. Chung. "Tim Hunt, Sexism and Science: The Real 'Trouble With Girls' in Labs." *CBC News Technology and Science*, June 12, 2015. http://www.cbc.ca/news/technology/ti...labs-1.3110133. Accessed 8/4/2016.
10. 10 American Association of University Women. "Building a STEM Pipeline for Girls and Women." www.aauw.org/what-we-do/stem-education/. Accessed June 10, 2016.
11. 11 National Aeronautics and Space Administration. "Outreach Programs: Women and Girls Initiative." http://women.nasa.gov/outreach-programs/. Accessed June 10, 2016.

This page titled 15.1: DNA Structure is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by OpenStax via source content that was edited to the style and standards of the LibreTexts platform.

- **10.2: Structure and Function of DNA** by OpenStax is licensed CC BY 4.0. Original source: https://openstax.org/details/books/microbiology.

15.2: Case Study- Decoding Disease - The Role of DNA Structure in Genetic Disorders

Introduction: Molecular genetics provides the blueprint for understanding how genetic information is encoded and expressed in all living organisms. Central to this field is DNA, the molecule that holds the code for inherited traits and the potential for genetic disorders. This case study explores the role of genetic counselors in explaining the implications of DNA structure changes to individuals at risk for genetic disorders.

Scenario: At GenLife Institute, genetic counselors like Sarah Bennett play a crucial role in helping patients understand their genetic makeup. Sarah is currently working with a family who has a history of a rare genetic disorder. She uses models and diagrams to explain the structure of DNA and how specific changes in DNA can lead to the health challenges they are concerned about.

DNA Structure and Its Components: Sarah begins by explaining that DNA is a double helix composed of nucleotides, each containing a sugar molecule, a phosphate group, and a nitrogenous base. She describes how the sequence of these bases along the DNA strand encodes the genetic instructions used in the development and functioning of all known living organisms and many viruses.

Case Study Questions:

1. **Describe the structure of DNA and its components.**
2. **How do mutations in DNA contribute to genetic diseases?**

Hands-On Classroom Activities:

1. **DNA Mutation Model:** In the "DNA Mutation Model" activity, students will physically manipulate models of DNA strands to introduce mutations and then engage in discussions about how these alterations can lead to genetic disorders and impact an organism's health.

Conclusion: Sarah's guidance helps the family to understand the complex nature of DNA and the impact of its structure on their health. By elucidating the connection between DNA mutations and genetic disorders, genetic counselors like Sarah enable patients to make informed decisions about their health and family planning. This case study highlights the critical role of molecular genetics in disease comprehension and the invaluable expertise that genetic counselors provide in interpreting this information for individuals and families facing genetic health risks.

15.2: Case Study- Decoding Disease - The Role of DNA Structure in Genetic Disorders is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

15.E: Exercises

Multiple Choice

1. A nucleic acid is:

    a) a polymer of nucleotides

    b) hydrophobic

    c) linked to an amino acid via a peptide bond

    d) a form of energy storage in the cell

2. Which could be a nucleotide base sequence in DNA?

    a) CAUGG

    b) AUGGA

    c) ACGTA

    d) USGGA

3. One unique property of DNA is its ability to

    a) reproduce

    b) catalyze

    c) replicate

    d) metabolize

4. Two nucleotides on the same strand of DNA are held together by

    a) peptide bonds

    b) hydrogen bonds

    c) disulfide bonds

    d) phosphodiester bonds

5. There are ___ codons but they code for only ___ amino acids.

    a) 20, 64

    b) 64, 20

    c) 63, 20

    d) 61, 20

6. The process by which DNA is converted into RNA is called

    a) replication

    b) transcription

    c) translation

    d) reverse transcription

7. Which of the following is not a constituent of deoxyribonucleotides?

    a) phosphate

    b) deoxyribose

    c) ribose

d) organic bases

8. Which base pair typically occurs in double-stranded DNA?

a) G-C

b) G-T

c) G-A

d) G-G

9. Which structural property of DNA is crucial for the conservation of genetic information?

a) antiparallel strands

b) the ability to form a double helix

c) base-pair complementarity

d) all of the above

10. Which of the following is not a characteristic of DNA?

a) double-stranded helix

b) composed of nucleotides

c) contains glucose

d) antiparallel strands

11. Which of the following is not a base used in DNA?

a) thymine

b) uracil

c) guanine

d) adenine

12. A molecule with the formula $C_{196}H_{245}N_{80}O_{115}P_{19}$ is most likely a(n):

a) peptide

b) nucleotide

c) oligonucleotide

d) chromosome

Warm-Up Questions

1. Nucleotides are to nucleic acids as _____ are to proteins.

2. Pyrimidine bases are used in both RNA and DNA structures, but the base _____ is used exclusively in DNA.

3. What is the difference between a nucleoside and a nucleotide?

4. What is a nucleotide base pair?

5. Write the sequence that complements the sequence 5'-A-T-T-C-C-G-T-C-A-G-3' in double-stranded DNA.

6. Write the sequence that complements the sequence 5'-C-C-G-T-T-A-A-T-G-C-3' in double-stranded DNA.

7. Write the RNA sequence that is encoded by the DNA sequence 5'-G-C-T-A-A-T-G-G-C-C-3'

8. Write the RNA sequence that is encoded by the DNA sequence 5'-T-A-G-C-G-T-T-A-C-G-3'

Intermediate Questions

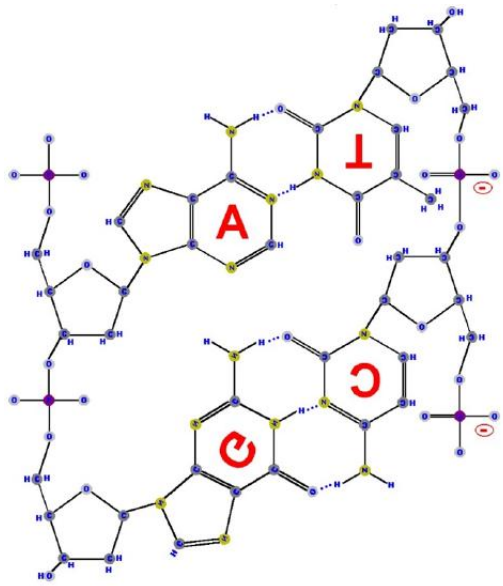
1. Write the amino acid sequence that is encoded by the DNA sequence 5'-GCAGGCAAACCATTTGAATGA-3'

2. Write the amino acid sequence that is encoded by the DNA sequence 5'-AATCGTTCTGAATCT-3"

3. How are carbohydrates involved in the structure of nucleic acids, and what specific sugar is found in these molecules?

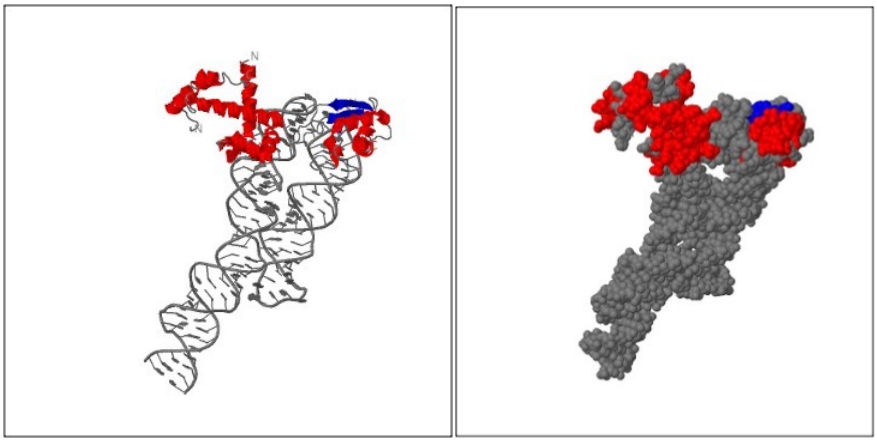
4. Explain what it means for the DNA strands in a double helix to be "antiparallel".

5. In the image below, indicate the location of phosphodiester bonds, purines, pyrimidines and hydrogen bonds.



http://www.synapses.co.uk/genetics/atandgc.gif

6. The images below show ribbon (left) and space-fill (right) models for a large molecular complex. Describe the types of molecules that are included.



Challenge Questions

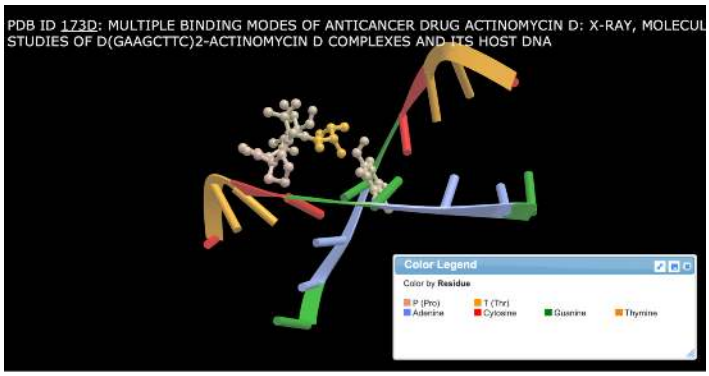
1. Explain the structural properties of double-stranded DNA that allow it to denature (melt) and renature without changing the genetic sequence.

2. Growing organisms devote a lot of their energy to DNA synthesis. Explain the role of deoxynucleotide triphosphates (dNTPs, the building blocks of DNA) in providing this energy.

Health-Related Questions

1. Ultraviolet radiation (such as from sunlight) can affect DNA by linking adjacent pyrimidine bases together or by causing G to be converted to T through oxidation reactions. What are the effects of these chemical changes on DNA structure and information content?

2. Actinomycin was the earliest identified member of a class of antibiotics called DNA intercalators. Members of this class are also potent anti-cancer drugs. Refer to the image below, and follow the link to view an interactive 3-D representation of actinomycin bound to DNA. Use the toolbar at the top of the page to change the way protein and nucleic acid components are displayed. Comment on the amino acids shown in the protein, its structure, and its position relative to the DNA double helix. Given what you know about DNA structure, what effect will the presence of actinomycin have on other DNA-binding proteins?



https://www.ncbi.nlm.nih.gov/Structure/icn3d/full.html?mmdbid=173d

---

15.E: Exercises is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

CHAPTER OVERVIEW

16: Answers to Odd Problems

16.1: Ch. 1 Odd Answers
16.2: Ch. 2 Odd Answers
16.3: Ch. 3 Odd Answers
16.4: Ch. 4 Odd Answers
16.5: Ch. 5 Odd Answers
16.6: Ch. 6 Odd Answers
16.7: Ch. 7 Odd Answers
16.8: Ch. 8 Odd Answers
16.9: Ch. 9 Odd Answers
16.10: Ch. 10 Odd Answers
16.11: Ch. 11 Odd Answers
16.12: Ch. 12 Odd Answers
16.13: Ch. 13 Odd Answers
16.14: Ch. 14 Odd Answers
16.15: Ch. 15 Odd Answers

16: Answers to Odd Problems is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.1: Ch. 1 Odd Answers

Multiple Choice Questions

1. a

2. d

3. c

4. b

5. a

6. d

7. b

8. d

9. a

10. c

Warm-up Problems

1. a) 2.5×10^{-8} b) 4.468241×10^{6}

3. a) 1.342 km b) 3.58 ms

5. a) 4 b) 2

7. a) 8.14×10^{4} b) 2.35×10^{-2}

9. Wine is a mixture of ethyl alcohol and water.

11. Seawater is a homogeneous mixture because the makeup of the ocean in one location should be the same as the makeup of the ocean in another location.

Problems

1. 3.9 mg

3. 8.4

5. 37.0 °C

7. 5.8 g water

Challenge Problems

1. 39.7

3. 0.3250 g

Health-related Problems

1. 25 mcg of fentanyl

3. 36.8 °C, 38.2 °C

5. Blood is a heterogeneous mixture.

16.1: Ch. 1 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.2: Ch. 2 Odd Answers

Multiple Choice Questions

1. a

2. c

3. a

4. c

5. d

6. d

7. a

8. b

9. c

10. a

Warm-up Problems

1. a) potassium b) carbon c) barium d) aluminum

3. 15 protons, 16 neutrons, 18 electrons

5. $^{34}S^{2-}$

7. 4 valence electrons

9. a) Na b) Cl c) P

11. As, Kr, P, Cl

Problems

1. Because there are only two stable isotopes, the average mass will be closer to the mass of the more abundant isotope, which means ^{193}Ir is more abundant.

3. fluorine

5. The ionization energy of chlorine is smaller than that of fluorine because chlorine has a smaller effective nuclear charge as seen by its larger size.

7. oxygen = 1, carbon = 2, beryllium = 3

9. Phosphorus is more metallic than oxygen because it has a lower attraction for electrons due to its lower electronegativity. In general, metallic character increases as you move down and to the left on the periodic table.

Challenge Problems

1. Fluorine is highly electronegative and has 7 valence electrons. Because of this, fluorine is likely to accept a single electron in an ionic bond to fill its octet.

Health-related Problems

1. 43 protons, 56 neutrons, 43 electrons

3. alkaline earth metals

5. 9 protons, 9 neutrons, 10 electrons

16.2: Ch. 2 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.3: Ch. 3 Odd Answers

Multiple Choice Questions

1. d
2. b
3. d
4. b
5. a
6. a
7. b
8. c
9. d
10. d

Warm-up Problems

1. sodium, potassium, calcium, magnesium
3. lithium
5. $MgCl_2$
7. Conductivity is a physical property associated with metals.
9. 2+
11. covalent compound

Problems

1. a) cesium chloride b) barium oxide
3. a) hydrogen bromide b) aluminum fluoride
5. a) boron trichloride b) hydrogen selenide
7. a) ClO_2 b) N_2O_4 c) K_3P
9. a) $BaCl_2$ b) Mg_3N_2 c) SO_2
11. a) chromium(III) oxide b) iron(II) chloride c) chromium(III) oxide
13. a) nickel(II) carbonate b) molybdenum(VI) oxide c) cobalt(II) nitrate
15. a) K_3PO_4 b) $CuSO_4$ c) $CaCl_2$
17. a) calcium dihydrogen phosphate b) iron(II) sulfate c) calcium carbonate

Challenge Problems

1. Al_2O_3; Ga_2S_3
3. iron(III) sulfate, Fe^{3+}, SO_4^{2-}

Health-related Problem

1. CaC_2O_4; $Ca_3(PO_4)_2$. Both are ionic compounds.

16.3: Ch. 3 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.4: Ch. 4 Odd Answers

16.4: Ch. 4 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.5: Ch. 5 Odd Answers

16.5: Ch. 5 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.6: Ch. 6 Odd Answers

Multiple Choice Questions

1. a
2. b
3. d
4. b
5. d
6. b
7. c
8. a
9. b
10. b

Warm-up Problems

1. 1.2×10^{24} peas
3. 72.149 amu
5. 58.442 amu
7. 0.555 mol
9. 2.0×10^{-3} g or 2.0 mg

Problems

1. 108.010 amu
3. 163.941 amu
5. 42 mol
7. 3.0×10^{2} g
9. 0.428 mol
11. 9.70×10^{-4} mol

Challenge Problem

1. 15.9 µL

16.6: Ch. 6 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.7: Ch. 7 Odd Answers

Multiple Choice Questions

1. d

2. a

3. c

4. d

5. d

6. a

7. b

8. c

9. d

10. b

Warm-up Problems

1. a) 1, 1, 1, 2 b) 1, 4, 1, 2, 2

3. a) 2, 2, 2, 1 b) 1, 1, 1, 4

5. a) 4, 2, 1, 2, 2 b) 1, 5, 1

7. a) 1, 3, 1 b) 1, 4, 3

9. Increase N_2 concentration, increase H_2 concentration, increase the temperature, decrease the volume of the container.

Problems

1. a) CaCO3(s) à CaO(s) + CO2(g) b) 2C4H10(g) + 13O2(g) à 8CO2(g) + 10H2O(g)

3. a) 2KClO3(s) à 2KCl(s) + 3O2(g) b) 2Al(s) + 3I2(s) àAl2I6(s)

5. a) Ba(NO3)2, KClO3

   b) 2KClO3(s) à 2KCl(s) + 3O2(g)

   c) 2Ba(NO3)2(s) à 2BaO(s) + 2N2(g) + 5O2(g)

7. a) An increase in temperature will shift this equilibrium to the right. A decrease in volume will shift this equilibrium to the left.

   b) An increase in temperature will shift this equilibrium to the right. A decrease in volume will not cause this equilibrium to shift.

   c) An increase in temperature will shift this equilibrium to the left. A decrease in volume will not cause this equilibrium to shift.

   d) An increase in temperature will shift this equilibrium to the left. A decrease in volume will shift this equilibrium to the right.

9. a) no b) yes c) no

Challenge Problems

1. a) $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$

   b) $CaO(s) + H_2O(l) \rightarrow Ca(OH)_2(s)$

   c) $Ca(OH)_2(s) + MgCl_2(aq) \rightarrow Mg(OH)_2(s) + CaCl_2(aq)$

   d) $Mg(OH)_2(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + 2H_2O(l)$

   e) $MgCl_2(aq) \rightarrow Mg(s) + Cl_2(g)$

Health-related Problems

1. $C_6H_{12}O_6(s) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$

3. $3NaHCO_3(aq) + H_3C_6H_5O_7(aq) \rightarrow 3CO_2(g) + Na_3C_6H_5O_7(aq) + 3H_2O(l)$

16.7: Ch. 7 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.8: Ch. 8 Odd Answers

16.8: Ch. 8 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.9: Ch. 9 Odd Answers

16.9: Ch. 9 Odd Answers is shared under a CC BY 4.0 license and was authored, remixed, and/or curated by LibreTexts.

16.10: Ch. 10 Odd Answers

16.10: Ch. 10 Odd Answers is shared under a not declared license and was authored, remixed, and/or curated by LibreTexts.

16.11: Ch. 11 Odd Answers

16.11: Ch. 11 Odd Answers is shared under a not declared license and was authored, remixed, and/or curated by LibreTexts.

16.12: Ch. 12 Odd Answers

Multiple Choice Questions

1. b
2. c
3. b
4. c
5. c
6. d
7. b
8. b
9. c
10. a

Warm-up Problems

1. condensation; hydrolysis

3. monosaccharide (sorbose)

5. disaccharide (leucrose)

7. Left - (L) glucose, right - (D) glucose. The isomers are distinguished by the orientation of the hydroxyl group attached to the chiral carbon furthest from the carbonyl group.

Problems

1. The image shows a repeated unit of the chitin polysaccharide, containing beta 1à4 glycosidic bonds between two *N*-acetylglucosamine monosaccharides. Portions of the glycosidic bonds are shown on the left and right sides.

3. Glucose and fructose are linked through a C1-C2 glycosidic bond. This linkage orients the rings perpendicular to each other.

5. aldose-ketose

7. anomers

Challenge Problem

1. Both contain a hexose sugar in ring form. Glucose is an aldohexose containing only hydroxyl groups. The glucosamine sugar in muramic acid is also a 6-member hexose ring but has an amino group on C2 instead of a hydroxyl group. The 3-carbon molecule lactic acid is connected to the glucosamine through an ester bond on C3.

Health-Related Question

1. Diabetes mellitus is characterized by high blood sugar. At higher concentrations of glucose, more glycosylated hemoglobin is formed and circulates in the bloodstream. Levels of hemoglobin A1c change over time but do not fluctuate like blood glucose levels, making hemoglobin A1c a good indicator of diabetes treatment effectiveness over the long term.

16.12: Ch. 12 Odd Answers is shared under a not declared license and was authored, remixed, and/or curated by LibreTexts.

16.13: Ch. 13 Odd Answers

Multiple choice Questions

1. b
2. a
3. b
4. c
5. d
6. a
7. c
8. b
9. c
10. d
11. a
12. c
13. b
14. a

Warm-Up Problems

1. butyric acid - short-chain, saturated fatty acid

3. arachidonic acid - long-chain, polyunsaturated fatty acid

Matching:

1. Triglyceride - D. Lipid molecule composed of a glycerol backbone and three fatty acid chains
2. Phospholipid - B. Component of cell membranes
3. Small intestine - C. Lipid digestion begins here
4. Saturated fatty acid - J. Lipid molecule with no carbon-carbon double bonds in the fatty acid chains
5. Cholesterol - G. Lipid molecule important for hormone synthesis
6. Unsaturated fatty acid - F. Lipid molecule with carbon-carbon double bonds in the fatty acid chains
7. Omega-3 fatty acids - 7. Lipid molecule important for hormone synthesis
8. Lipoproteins - H. Lipid carrier proteins in the bloodstream
9. LDL (Low-Density Lipoprotein) and HDL (High-Density Lipoprotein) - I. Lipid that can be classified as LDL or HDL
10. Chylomicrons - A. Lipid primarily used for long-term energy storage

Problems

1. The abundance of oxygen in the molecule is the major determinant of its structure and classification. In carbohydrates, the ratio of hydrogen to oxygen is typically 2:1 (as in the water molecule) and most carbons are bonded to at least one oxygen in a hydroxyl, carbonyl or ester. In lipids, the ratio of hydrogen to oxygen is much higher and carbon-oxygen bonds are found only in certain portions of the molecule.

3. Linoleic acid is a polyunsaturated fatty acid containing two *cis* double bonds along an 18-carbon chain. The *cis* double bonds cause the chain to be kinked and bend back on itself.

5. Lipids are transported through the bloodstream, stored in adipose tissue, and can be broken down into fatty acids and glycerol to provide energy when needed.

7. Lipids are mostly hydrophobic, meaning that they will avoid water and will not dissolve in aqueous solutions. They will disperse in non-polar organic solvents such as acetone and benzene.

Challenge Problem

1. Differences in shape between large hydrophobic sections and polar headgroups means lipids will fit together in different ways. Closely packed hydrophobic sections with saturated or trans-unsaturated tails will be less fluid. Loosely packed hydrophobic sections with cis unsaturated tails will be more fluid.

Health-Related Question

1. HDL particles contain a mixture of lipids. Amphipathic lipids including phospholipids and unesterified cholesterol form a micellar structure. Hydrophobic triglycerides and cholesteryl ester (cholesterol esterified to a fatty acyl chain) are in the interior of the micelle. In addition, the HDL particle contains a protein component, apolipoprotein A1, which is embedded into the micellar lipid monolayer.

16.13: Ch. 13 Odd Answers is shared under a not declared license and was authored, remixed, and/or curated by LibreTexts.

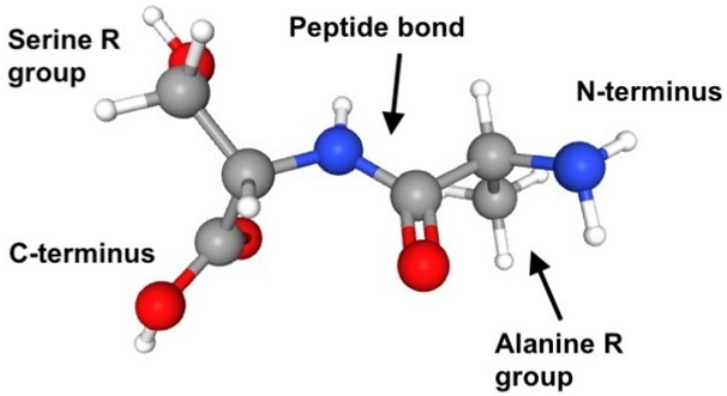
16.14: Ch. 14 Odd Answers

Multiple Choice Questions

1. c
2. b
3. b
4. d
5. d
6. c
7. a
8. b
9. d
10. d
11. d
12. a
13. b
14. a

Warm-Up Problems

1. Phenylalanine
3. Histidine
5. Tryptophan
7.



Problems

1. Proline contains a ring structure that connects its side chain to the carbon-carbon-nitrogen backbone. The rigid ring structure affects the overall protein structure because the peptide chains are “kinked” and less flexible in regions where prolines are present. These features make proline an important driver of protein structure by disallowing certain configurations.

3. *Answers will vary*

5. +1 (Met -NH3), +1 (Arg), -1 (Glu), +1 (Lys), -1 (Lys -COOH) = **+1**

7. Single polypeptide with tertiary structure, two major domains, secondary structure includes beta strands/sheets in both domains and alpha helices (mostly in lower domain).

Challenge Problems

1. Channel proteins span the length of a lipid bilayer and allow polar molecules like ions and water to pass through membranes. The “ends” of the protein and the channel interior will have mostly polar, uncharged amino acid side chains. Some charged side chains like lysine and arginine will be used to form a narrow pore for the ions to pass through. The exterior of the protein is embedded in the lipid bilayer next to fatty acid chain and will consist of hydrophobic amino acids like alanine and valine.

Health-Related Problem

1. Each new protein folds into its functional conformation (shape) under a range of thermodynamically favorable conditions. When temperature and pH change, the increased movement due to excess thermal energy and the changes in side-chain electric charge can affect the non-covalent bonds between portions of the polypeptide. This can lead to an un-ordered or disordered protein conformation and prevent proper function.

16.14: Ch. 14 Odd Answers is shared under a not declared license and was authored, remixed, and/or curated by LibreTexts.

16.15: Ch. 15 Odd Answers

Multiple Choice Questions

1. a

2. c

3. c

4. d

5. b

6. b

7. c

8. a

9. d

10. c

11. b

12. c

Warm-Up Problems

1.amino acids

3. Nucleosides contain a base and a sugar without a phosphate. Nucleotides are nucleosides that have one, two, or three phosphate groups esterified at the 5' hydroxyl.

5. 3’-T-A-A-G-G-C-A-G-T-C-5’ or 5’-C-T-G-A-C-G-G-A-A-T-3’

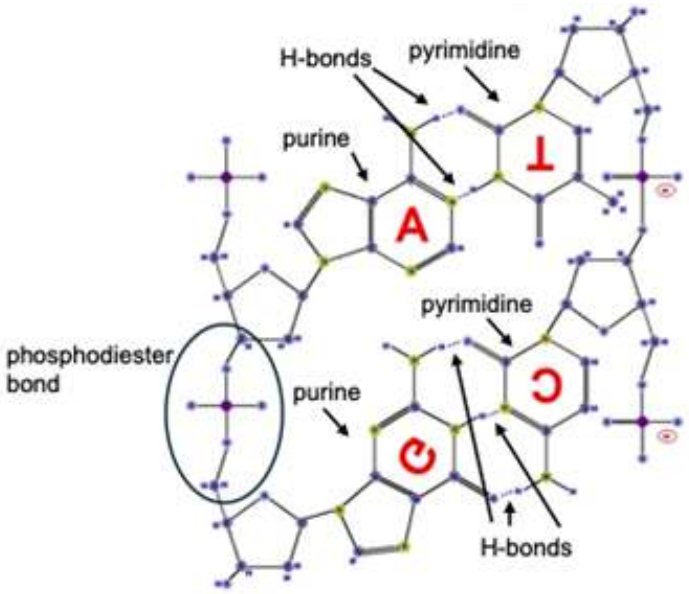
7. 5’-G-C-U-A-A-U-G-G-C-C-3’

Problems

1. A G K P F E stop

3. The pentose sugars ribose and deoxyribose are part of the nucleotides that are building blocks for RNA and DNA, respectively. The nitrogen bases are covalently linked to and are co-planar with the sugars.

5.



Challenge Problems

1. The hydrogen bonds between nitrogenous bases are weaker than the covalent ester bonds in the sugar-phosphate backbone and can be disrupted through thermal and chemical denaturants.

Health-Related Question

1. Pyrimidine bases are normally paired with purine bases through hydrogen bonds. The formation of a pyrimidine dimer (covalently bonded T-T or C-C pairs) will introduce a “kink” in the DNA double helix that can prevent the DNA replication or transcription machinery from reading the code correctly. The same is true for a chemical modification that causes a G base to be read as a T. If the damage is not repaired, the cell may die or acquire a mutation in an important region of the genome.

16.15: Ch. 15 Odd Answers is shared under a not declared license and was authored, remixed, and/or curated by LibreTexts.

Index

A

absolute zero
8.3: The Gas Laws
accuracy
5.2: Measurement Uncertainty, Accuracy, and Precision
acid ionization
9.1: What are Acids and Bases?
acidic
9.2: pH and pOH
adenine
15.1: DNA Structure
alcohol
11.2: Alcohols and Ethers
aldehyde
11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters
alloy
8.5: Types of Solutions
amide
11.4: Amines and Amides
amine
11.4: Amines and Amides
Amino acid
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
Amonton's law
8.3: The Gas Laws
amphiprotic
9.1: What are Acids and Bases?
amphoteric
9.1: What are Acids and Bases?
antiparallel
15.1: DNA Structure
aqueous solution
8.7: Concentration
atmosphere
8.2: Gas Pressure
atom
1.3: Matter
atomic mass
2.2.1: Nuclei of Atoms
autoionization
9.1: What are Acids and Bases?
Avogadro's law
8.3: The Gas Laws
Avogadro's number
6.1: The Mole
6.2: Formula Mass
6.3: Converting between Grams and Moles
axial position
4.3: Molecular Structure and Polarity

B

balanced equation
7.1: Balancing Chemical Equations
bar
8.2: Gas Pressure
barometer
8.2: Gas Pressure
base ionization
9.1: What are Acids and Bases?
basic
9.2: pH and pOH
binary acid
3.4: Chemical Nomenclature
binary compound
3.4: Chemical Nomenclature
boiling point elevation
8.8: Osmosis, Diffusion and Dialysis
boiling point elevation constant
8.8: Osmosis, Diffusion and Dialysis
bond angle
4.3: Molecular Structure and Polarity
bond dipole moment
4.3: Molecular Structure and Polarity
bond distance
4.3: Molecular Structure and Polarity
bond length
3.3: Covalent Bonding
Boyle's law
8.3: The Gas Laws

C

calorie
7.2: Energy Basics
carbohydrate
12.1: Carbohydrates
carbonyl group
11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters
carboxylic acid
11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters
cellulose
12.1: Carbohydrates
Celsius
1.2: Units
5.1: Density and Temperature
Chaperones
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
Charles's law
8.3: The Gas Laws
chemical change
1.4: Physical and Chemical Properties
chemical equation
7.1: Balancing Chemical Equations
chemical property
1.4: Physical and Chemical Properties
chemistry
1.1: The Scientific Method
2: Atoms and Elements
3: Ionic and Covalent Compounds
chitin
12.1: Carbohydrates
coefficient
7.1: Balancing Chemical Equations
colligative property
8.8: Osmosis, Diffusion and Dialysis
complete ionic equation
7.1: Balancing Chemical Equations
compound
1.3: Matter
concentrated
8.7: Concentration
concentration
8.7: Concentration
conjugate acid
9.1: What are Acids and Bases?
conjugate base
9.1: What are Acids and Bases?
conversion factors
5.1.1: Mathematical Treatment of Measurement Results
5.3: Unit Conversions
covalent bond
3.1: Molecular and Ionic Compounds
3.3: Covalent Bonding
covalent compound
3.1: Molecular and Ionic Compounds
crenation
8.8: Osmosis, Diffusion and Dialysis
cubic centimeter
1.2: Units
5.1: Density and Temperature
cubic meter
1.2: Units
5.1: Density and Temperature
cytosine
15.1: DNA Structure

D

denaturation
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
density
1.2: Units
5.1: Density and Temperature
Deoxyribonucleotides
15.1: DNA Structure
deoxyribose
15.1: DNA Structure
dilution
8.7: Concentration
dimensional analysis
5.1.1: Mathematical Treatment of Measurement Results
5.3: Unit Conversions
dipole moment
4.3: Molecular Structure and Polarity
Disaccharide
12.1: Carbohydrates
Dispersion
8.4: Intermolecular Forces
dissociation
8.6: Electrolytes
dissolved
8.7: Concentration

double bond
4.1: Lewis Symbols and Structures

E

electrolyte
8.6: Electrolytes
electronegativity
3.3: Covalent Bonding
element
1.3: Matter
Elements for Life
2.6: Health Connections- Essential Elements for Life
endothermic process
7.2: Energy Basics
energy
7.2: Energy Basics
enzyme
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
equatorial position
4.3: Molecular Structure and Polarity
Essential Elements
2.6: Health Connections- Essential Elements for Life
ester
11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters
ether
11.2: Alcohols and Ethers
exact number
5.2: Measurement Uncertainty, Accuracy, and Precision
exothermic process
7.2: Energy Basics
extensive property
1.4: Physical and Chemical Properties

F

Fahrenheit
5.1.1: Mathematical Treatment of Measurement Results
5.3: Unit Conversions
formal charge
4.2: Formal Charges and Resonance
formula mass
6.1: The Mole
6.2: Formula Mass
6.3: Converting between Grams and Moles
free radical
4.1: Lewis Symbols and Structures
freezing point depression
8.8: Osmosis, Diffusion and Dialysis
freezing point depression constant
8.8: Osmosis, Diffusion and Dialysis

G

gas
1.3: Matter
glycogen
12.1: Carbohydrates
glycosidic bond
12.1: Carbohydrates
guanine
15.1: DNA Structure

H

heat
7.2: Energy Basics
heat capacity
7.2: Energy Basics
hemolysis
8.8: Osmosis, Diffusion and Dialysis
heterogeneous catalyst
7.4: Catalysis
heterogeneous mixture
1.3: Matter
homogeneous catalyst
7.4: Catalysis
homogeneous mixture
1.3: Matter
hormone
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
hybrid orbital
4.5: Hybrid Atomic Orbitals
hybridization
4.5: Hybrid Atomic Orbitals
hydrogen bonding
8.4: Intermolecular Forces
hydrostatic pressure
8.2: Gas Pressure
hypercapnia
9.3: Acid-Base Balance
hypertonic
8.8: Osmosis, Diffusion and Dialysis
hypervalent molecule
4.1: Lewis Symbols and Structures
hypothesis
1.1: The Scientific Method
2: Atoms and Elements
3: Ionic and Covalent Compounds
hypotonic
8.8: Osmosis, Diffusion and Dialysis

I

ideal gas
8.3: The Gas Laws
ideal gas constant
8.3: The Gas Laws
ideal gas law
8.3: The Gas Laws
ideal solution
8.5: Types of Solutions
induced dipole
8.4: Intermolecular Forces
inert pair effect
3.2: Ionic Bonding
instantaneous dipole
8.4: Intermolecular Forces
intensive property
1.4: Physical and Chemical Properties
intermolecular force
8.4: Intermolecular Forces
International System of Units
1.2: Units
5.1: Density and Temperature
ion pair
8.8: Osmosis, Diffusion and Dialysis
ionic bond
3.1: Molecular and Ionic Compounds
3.2: Ionic Bonding
ionic compound
3.1: Molecular and Ionic Compounds
isotonic
8.8: Osmosis, Diffusion and Dialysis
isotopes
2.2.1: Nuclei of Atoms

J

joule
7.2: Energy Basics

K

kelvin
1.2: Units
5.1: Density and Temperature
ketone
11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters
kilogram
1.2: Units
5.1: Density and Temperature
kinetic energy
7.2: Energy Basics
kinetic molecular theory
8.1: The Kinetic-Molecular Theory

L

law
1.1: The Scientific Method
2: Atoms and Elements
3: Ionic and Covalent Compounds
law of conservation of matter
1.3: Matter
Le Châtelier's principle
7.3: Chemical Equilibrium
length
1.2: Units
5.1: Density and Temperature
Lewis structure
4.1: Lewis Symbols and Structures
Lewis symbol
4.1: Lewis Symbols and Structures
linear
4.3: Molecular Structure and Polarity
lipid
13.1: Lipids
liquid
1.3: Matter
liter
1.2: Units
5.1: Density and Temperature
lone pair
4.1: Lewis Symbols and Structures

M

macroscopic domain
- 1.1: The Scientific Method
- 2: Atoms and Elements
- 3: Ionic and Covalent Compounds

manometer
- 8.2: Gas Pressure

mass
- 1.3: Matter

mass percentage
- 8.7.1: Other Units for Solution Concentrations

meter
- 1.2: Units
- 5.1: Density and Temperature

microscopic domain
- 1.1: The Scientific Method
- 2: Atoms and Elements
- 3: Ionic and Covalent Compounds

milliliter
- 1.2: Units
- 5.1: Density and Temperature

mixture
- 1.3: Matter

molality
- 8.8: Osmosis, Diffusion and Dialysis

molar mass
- 6.1: The Mole
- 6.2: Formula Mass
- 6.3: Converting between Grams and Moles

molarity
- 8.7: Concentration

mole
- 6.1: The Mole
- 6.2: Formula Mass
- 6.3: Converting between Grams and Moles

molecular compound
- 3.1: Molecular and Ionic Compounds

molecular equation
- 7.1: Balancing Chemical Equations

molecular structure
- 4.2: Formal Charges and Resonance
- 4.3: Molecular Structure and Polarity

molecule
- 1.3: Matter

monatomic ion
- 3.1: Molecular and Ionic Compounds

Monosaccharide
- 12.1: Carbohydrates

N

net ionic equation
- 7.1: Balancing Chemical Equations

neutral
- 9.2: pH and pOH

nitrogenous base
- 15.1: DNA Structure

node
- 4.4: Valence Bond Theory

nomenclature
- 3.4: Chemical Nomenclature

nonelectrolyte
- 8.6: Electrolytes

nonpolar covalent bond
- 3.3: Covalent Bonding

nucleic acids
- 15.1: DNA Structure

nucleotides
- 15.1: DNA Structure

O

octahedral
- 4.3: Molecular Structure and Polarity

octet rule
- 4.1: Lewis Symbols and Structures

omega fat
- 13.1: Lipids

osmosis
- 8.8: Osmosis, Diffusion and Dialysis

osmotic pressure
- 8.8: Osmosis, Diffusion and Dialysis

overlap
- 4.4: Valence Bond Theory

oxyacid
- 3.4: Chemical Nomenclature

oxyanion
- 3.1: Molecular and Ionic Compounds

P

parts per billion
- 8.7.1: Other Units for Solution Concentrations

parts per million
- 8.7.1: Other Units for Solution Concentrations

pascal
- 8.2: Gas Pressure

Peptide bond
- 14.1: Properties of Proteins
- 14.2: Amino Acids
- 14.3: Primary Structure- Peptides
- 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins

pH
- 9.2: pH and pOH

phosphodiester backbones
- 15.1: DNA Structure

phospholipid
- 13.1: Lipids

physical change
- 1.4: Physical and Chemical Properties

physical property
- 1.4: Physical and Chemical Properties

pi bond
- 4.4: Valence Bond Theory

plasma
- 1.3: Matter

pOH
- 9.2: pH and pOH

polar covalent bond
- 3.3: Covalent Bonding

polar molecule
- 4.3: Molecular Structure and Polarity

Polarizability
- 8.4: Intermolecular Forces

polyatomic ion
- 3.1: Molecular and Ionic Compounds

polypeptide
- 14.1: Properties of Proteins
- 14.2: Amino Acids
- 14.3: Primary Structure- Peptides
- 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins

polysaccharide
- 12.1: Carbohydrates

position of equilibrium
- 7.3: Chemical Equilibrium

potential energy
- 7.2: Energy Basics

pounds per square inch
- 8.2: Gas Pressure

precision
- 5.2: Measurement Uncertainty, Accuracy, and Precision

pressure
- 8.2: Gas Pressure

primary structure
- 14.1: Properties of Proteins
- 14.2: Amino Acids
- 14.3: Primary Structure- Peptides
- 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins

product
- 7.1: Balancing Chemical Equations

protein
- 14.1: Properties of Proteins
- 14.2: Amino Acids
- 14.3: Primary Structure- Peptides
- 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins

PSI (Unit)
- 8.2: Gas Pressure

pure covalent bond
- 3.3: Covalent Bonding

pure substance
- 1.3: Matter

purines
- 15.1: DNA Structure

pyrimidines
- 15.1: DNA Structure

Q

quaternary structure
- 14.1: Properties of Proteins
- 14.2: Amino Acids
- 14.3: Primary Structure- Peptides
- 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins

R

Raoult's law
- 8.8: Osmosis, Diffusion and Dialysis

reactant
- 7.1: Balancing Chemical Equations

resonance
- 4.2: Formal Charges and Resonance
- 4.6: Multiple Bonds

resonance forms
- 4.2: Formal Charges and Resonance

resonance hybrid
- 4.2: Formal Charges and Resonance

root mean square velocity
- 8.1: The Kinetic-Molecular Theory

rounding
5.2: Measurement Uncertainty, Accuracy, and Precision

S

Saturated fatty acid
13.1: Lipids
scientific method
1.1: The Scientific Method
2: Atoms and Elements
3: Ionic and Covalent Compounds
second
1.2: Units
5.1: Density and Temperature
secondary structure
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
semipermeable membrane
8.8: Osmosis, Diffusion and Dialysis
SI units
1.2: Units
5.1: Density and Temperature
sigma bond
4.4: Valence Bond Theory
significant figures
5.2: Measurement Uncertainty, Accuracy, and Precision
single bond
4.1: Lewis Symbols and Structures
solid
1.3: Matter
solute
8.7: Concentration
solvation
8.5: Types of Solutions
solvent
8.7: Concentration
sp hybrid orbital
4.5: Hybrid Atomic Orbitals
sp2 hybrid orbital
4.5: Hybrid Atomic Orbitals
sp3 hybrid orbital
4.5: Hybrid Atomic Orbitals
sp3d hybrid orbital
4.5: Hybrid Atomic Orbitals
sp3d2 hybrid orbital
4.5: Hybrid Atomic Orbitals
specific heat capacity
7.2: Energy Basics
spectator ion
7.1: Balancing Chemical Equations
spontaneous process
8.5: Types of Solutions
standard conditions of temperature and pressure
8.3: The Gas Laws
standard molar volume
8.3: The Gas Laws
starch
12.1: Carbohydrates
steroid
13.1: Lipids
STP
8.3: The Gas Laws
stress
7.3: Chemical Equilibrium
strong electrolyte
8.6: Electrolytes
symbolic domain
1.1: The Scientific Method
2: Atoms and Elements
3: Ionic and Covalent Compounds

T

temperature
7.2: Energy Basics
tertiary structure
14.1: Properties of Proteins
14.2: Amino Acids
14.3: Primary Structure- Peptides
14.4: Secondary, Tertiary, and Quaternary Structure of Proteins
tetrahedral
4.3: Molecular Structure and Polarity
theory
1.1: The Scientific Method
2: Atoms and Elements
3: Ionic and Covalent Compounds
thermal energy
7.2: Energy Basics
thermochemistry
7.2: Energy Basics
thymine
15.1: DNA Structure
torr
8.2: Gas Pressure
trans fat
13.1: Lipids
triacylglycerol
13.1: Lipids
triglyceride
13.1: Lipids
trigonal bipyramidal
4.3: Molecular Structure and Polarity
trigonal planar
4.3: Molecular Structure and Polarity
triple bond
4.1: Lewis Symbols and Structures

U

uncertainty
5.2: Measurement Uncertainty, Accuracy, and Precision
unit
1.2: Units
5.1: Density and Temperature
unsaturated fatty acid
13.1: Lipids

V

valence bond theory
4.4: Valence Bond Theory
valence shell electron pair repulsion theory
4.3: Molecular Structure and Polarity
van der Waals force
8.4: Intermolecular Forces
van't Hoff factor
8.8: Osmosis, Diffusion and Dialysis
vertical gene transfer
15.1: DNA Structure
volume
1.2: Units
5.1: Density and Temperature
volume percentage
8.7.1: Other Units for Solution Concentrations
VSEPR
4.3: Molecular Structure and Polarity

W

wax
13.1: Lipids
weak electrolyte
8.6: Electrolytes
weight
1.3: Matter
work
7.2: Energy Basics

Glossary

Sample Word 1 | Sample Definition 1

Detailed Licensing

Overview

Title: General, Organic, and Biochemistry with Problems, Case Studies, and Activities

Webpages: 136

All licenses found:

- CC BY 4.0: 94.1% (128 pages)
- Undeclared: 5.9% (8 pages)

By Page

- General, Organic, and Biochemistry with Problems, Case Studies, and Activities - *CC BY 4.0*
  - Front Matter - *CC BY 4.0*
    - TitlePage - *CC BY 4.0*
    - InfoPage - *CC BY 4.0*
    - Preface - *Undeclared*
    - Table of Contents - *Undeclared*
    - Licensing - *CC BY 4.0*
  - 1: Scientific Method, Matter, and Measurements - *CC BY 4.0*
    - 1.1: The Scientific Method - *CC BY 4.0*
    - 1.2: Units - *CC BY 4.0*
    - 1.3: Matter - *CC BY 4.0*
    - 1.4: Physical and Chemical Properties - *CC BY 4.0*
    - 1.5: Case Study- Using the Scientific Method to Diagnose an Autoimmune Disorder - *CC BY 4.0*
    - 1.E: Exercises - *CC BY 4.0*
  - 2: Atoms and Elements - *CC BY 4.0*
    - 2.1: Atomic Theory - *CC BY 4.0*
    - 2.2: Atomic Structure - *CC BY 4.0*
      - 2.2.1: Nuclei of Atoms - *CC BY 4.0*
    - 2.3: Atomic Masses - *CC BY 4.0*
    - 2.4: Electronic Structure in Atoms - *CC BY 4.0*
    - 2.5: The Periodic Table - *CC BY 4.0*
    - 2.6: Health Connections- Essential Elements for Life - *CC BY 4.0*
    - 2.7: Case Study- Electrons and Electronic Structure in Medical Applications - *CC BY 4.0*
    - 2.8: 3D Printing Activity - Periodic Trends - *CC BY 4.0*
    - 2.E: Exercises - *CC BY 4.0*
  - 3: Ionic and Covalent Compounds - *CC BY 4.0*
    - 3.1: Molecular and Ionic Compounds - *CC BY 4.0*
    - 3.2: Ionic Bonding - *CC BY 4.0*
    - 3.3: Covalent Bonding - *CC BY 4.0*
    - 3.4: Chemical Nomenclature - *CC BY 4.0*
    - 3.5: Case Study- Ionic and Covalent Compounds in Biochemistry - *CC BY 4.0*
    - 3.E: Exercises - *CC BY 4.0*
  - 4: Chemical Bonding - *CC BY 4.0*
    - 4.1: Lewis Symbols and Structures - *CC BY 4.0*
    - 4.2: Formal Charges and Resonance - *CC BY 4.0*
    - 4.3: Molecular Structure and Polarity - *CC BY 4.0*
    - 4.4: Valence Bond Theory - *CC BY 4.0*
    - 4.5: Hybrid Atomic Orbitals - *CC BY 4.0*
    - 4.6: Multiple Bonds - *CC BY 4.0*
    - 4.7: Case Study- Chemical Bonding - Deciphering Drug Interactions through Lewis Structures - *CC BY 4.0*
    - 4.8: 3D Printing Activity- VSEPR and Ionic/Metallic Solids Structures - *CC BY 4.0*
    - 4.E: Exercises - *CC BY 4.0*
  - 5: Unit Conversions - *CC BY 4.0*
    - 5.1: Density and Temperature - *CC BY 4.0*
      - 5.1.1: Mathematical Treatment of Measurement Results - *CC BY 4.0*
    - 5.2: Measurement Uncertainty, Accuracy, and Precision - *CC BY 4.0*
    - 5.3: Unit Conversions - *CC BY 4.0*
    - 5.4: Health Connections- Dosage Calculations - *CC BY 4.0*
    - 5.5: Case Study- Precision in Pediatric Care – The Imperative of Unit Conversion - *CC BY 4.0*
    - 5.E: Exercises - *CC BY 4.0*
  - 6: Moles - *CC BY 4.0*
    - 6.1: The Mole - *CC BY 4.0*
    - 6.2: Formula Mass - *CC BY 4.0*
    - 6.3: Converting between Grams and Moles - *CC BY 4.0*
    - 6.4: Case Study- The Mole Concept in Clinical Laboratory Analysis - *CC BY 4.0*
    - 6.E: Exercises - *CC BY 4.0*

- 7: Chemical Equations and Reactions - *CC BY 4.0*
  - 7.1: Balancing Chemical Equations - *CC BY 4.0*
  - 7.2: Energy Basics - *CC BY 4.0*
  - 7.3: Chemical Equilibrium - *CC BY 4.0*
  - 7.4: Catalysis - *CC BY 4.0*
  - 7.5: Case Study- Balancing Acts in Pharmacological Synthesis - *CC BY 4.0*
  - 7.E: Exercises - *CC BY 4.0*
- 8: Gases, Liquids, and Solids - *CC BY 4.0*
  - 8.1: The Kinetic-Molecular Theory - *CC BY 4.0*
  - 8.2: Gas Pressure - *CC BY 4.0*
  - 8.3: The Gas Laws - *CC BY 4.0*
  - 8.4: Intermolecular Forces - *CC BY 4.0*
  - 8.5: Types of Solutions - *CC BY 4.0*
  - 8.6: Electrolytes - *CC BY 4.0*
  - 8.7: Concentration - *CC BY 4.0*
    - 8.7.1: Other Units for Solution Concentrations - *CC BY 4.0*
  - 8.8: Osmosis, Diffusion and Dialysis - *CC BY 4.0*
  - 8.9: Health Connections- Oxygen in the Body - *CC BY 4.0*
  - 8.10: Case Study- The Vital Breath – Kinetic Molecular Theory in Respiratory Care - *CC BY 4.0*
  - 8.E: Exercises - *CC BY 4.0*
- 9: Acids and Bases - *CC BY 4.0*
  - 9.1: What are Acids and Bases? - *CC BY 4.0*
  - 9.2: pH and pOH - *CC BY 4.0*
  - 9.3: Acid-Base Balance - *CC BY 4.0*
  - 9.4: Case Study- Navigating the Delicate pH Spectrum in Intensive Care - *CC BY 4.0*
  - 9.E: Exercises - *CC BY 4.0*
- 10: Introduction to Organic Chemistry - *CC BY 4.0*
  - 10.1: Drawing organic structures - *CC BY 4.0*
  - 10.2: Alkanes and isomers - *CC BY 4.0*
  - 10.3: Functional groups - *CC BY 4.0*
  - 10.4: Case Study- The Molecular Tapestry of Healing - *CC BY 4.0*
  - 10.5: 3D Printing Activity- Cyclohexane - *CC BY 4.0*
  - 10.E: Exercises - *CC BY 4.0*
- 11: Organic Chemistry Reactions - *CC BY 4.0*
  - 11.1: Organic Reactions - *CC BY 4.0*
  - 11.2: Alcohols and Ethers - *CC BY 4.0*
  - 11.3: Aldehydes, Ketones, Carboxylic Acids, and Esters - *CC BY 4.0*
  - 11.4: Amines and Amides - *CC BY 4.0*
  - 11.E: Exercises - *CC BY 4.0*
- 12: Carbohydrates - *CC BY 4.0*
  - 12.1: Carbohydrates - *CC BY 4.0*
  - 12.2: Fischer and Haworth projections - *CC BY 4.0*
  - 12.3: Case Study- Tailoring Nutrition – Carbohydrates in Diabetes Care - *CC BY 4.0*
  - 12.E: Exercises - *CC BY 4.0*
- 13: Lipids - *CC BY 4.0*
  - 13.1: Lipids - *CC BY 4.0*
  - 13.2: Case Study- Lipids and Heart Health - Interpreting Lipid Profiles - *CC BY 4.0*
  - 13.E: Exercises - *CC BY 4.0*
- 14: Proteins - *CC BY 4.0*
  - 14.1: Properties of Proteins - *CC BY 4.0*
  - 14.2: Amino Acids - *CC BY 4.0*
  - 14.3: Primary Structure- Peptides - *CC BY 4.0*
  - 14.4: Secondary, Tertiary, and Quaternary Structure of Proteins - *CC BY 4.0*
  - 14.5: Case Study- Synergy in Science and Care - Protein Structures Illuminating Metabolic Disorder Management - *CC BY 4.0*
  - 14.6: 3D Printing Activity- Protein-Ligand Binding - *CC BY 4.0*
  - 14.E: Exercises - *CC BY 4.0*
- 15: Molecular Genetics - *CC BY 4.0*
  - 15.1: DNA Structure - *CC BY 4.0*
  - 15.2: Case Study- Decoding Disease - The Role of DNA Structure in Genetic Disorders - *CC BY 4.0*
  - 15.E: Exercises - *CC BY 4.0*
- 16: Answers to Odd Problems - *CC BY 4.0*
  - 16.1: Ch. 1 Odd Answers - *CC BY 4.0*
  - 16.2: Ch. 2 Odd Answers - *CC BY 4.0*
  - 16.3: Ch. 3 Odd Answers - *CC BY 4.0*
  - 16.4: Ch. 4 Odd Answers - *CC BY 4.0*
  - 16.5: Ch. 5 Odd Answers - *CC BY 4.0*
  - 16.6: Ch. 6 Odd Answers - *CC BY 4.0*
  - 16.7: Ch. 7 Odd Answers - *CC BY 4.0*
  - 16.8: Ch. 8 Odd Answers - *CC BY 4.0*
  - 16.9: Ch. 9 Odd Answers - *CC BY 4.0*
  - 16.10: Ch. 10 Odd Answers - *Undeclared*
  - 16.11: Ch. 11 Odd Answers - *Undeclared*
  - 16.12: Ch. 12 Odd Answers - *Undeclared*
  - 16.13: Ch. 13 Odd Answers - *Undeclared*
  - 16.14: Ch. 14 Odd Answers - *Undeclared*
  - 16.15: Ch. 15 Odd Answers - *Undeclared*
- Back Matter - *CC BY 4.0*
  - Index - *CC BY 4.0*
  - Glossary - *CC BY 4.0*
  - Detailed Licensing - *CC BY 4.0*