Organic Chemistry with Biological Topics

Sixth Edition

Janice Gorzynski Smith
University of Hawaiʻi at Mānoa

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ORGANIC CHEMISTRY WITH BIOLOGICAL TOPICS, SIXTH EDITION

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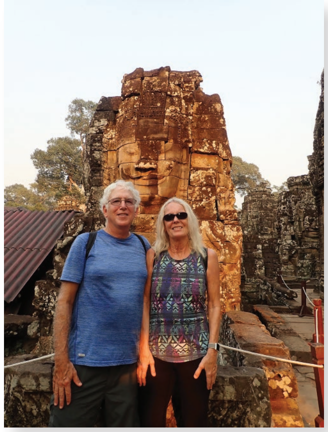
About the Author



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Janice Gorzynski Smith was born in Schenectady, New York. She received an A.B. degree *summa cum laude* in chemistry from Cornell University, and a Ph.D. in Organic Chemistry from Harvard University under the direction of Nobel Laureate E. J. Corey. During her tenure with the Corey group, she completed the total synthesis of the plant growth hormone gibberellic acid.

Following her postdoctoral work as a National Science Foundation National Needs Postdoctoral Fellow at Harvard, Jan joined the faculty of Mount Holyoke College, where she was employed for 21 years. During this time she was active in teaching organic chemistry lecture and lab courses, conducting a research program in organic synthesis, and serving as department chair. Her organic chemistry class was named one of Mount Holyoke's "Don't-miss courses" in a survey by *Boston* magazine. After spending two sabbaticals amidst the natural beauty and diversity in Hawai'i in the 1990s, Jan and her family moved there permanently in 2000. She has been a faculty member at the University of Hawai'i at Mānoa, where she has taught the two-semester organic chemistry lecture and lab courses. In 2003, she received the Chancellor's Citation for Meritorious Teaching.

Jan resides in Hawai'i with her husband Dan, an emergency medicine physician, pictured with her in Cambodia in 2018. She has four children and six grandchildren. When not teaching, writing, or enjoying her family, Jan bikes, hikes, snorkels, and scuba dives in sunny Hawai'i, and time permitting, enjoys travel and Hawaiian quilting.

For Megan Sarah

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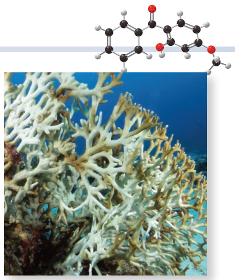

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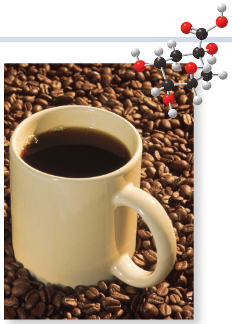

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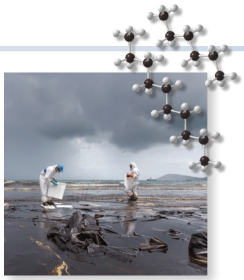

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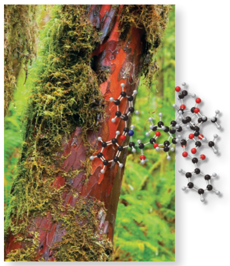

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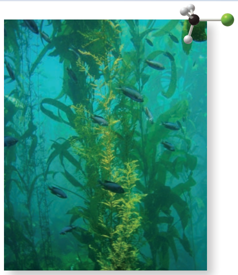

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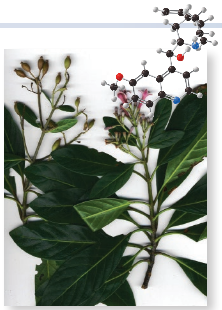

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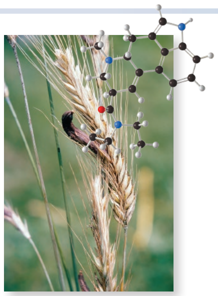

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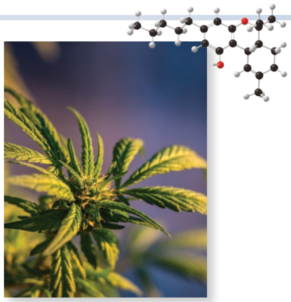

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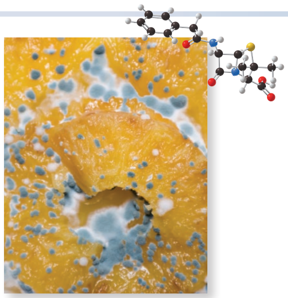

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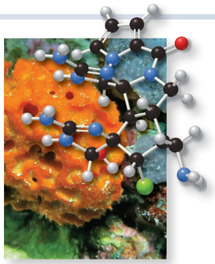

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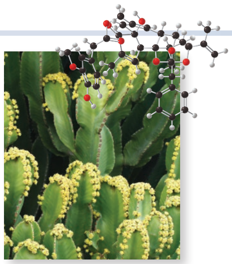

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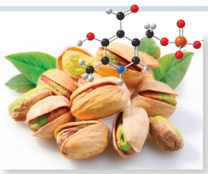

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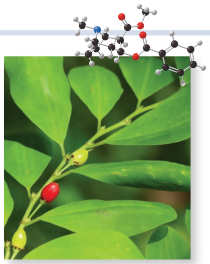

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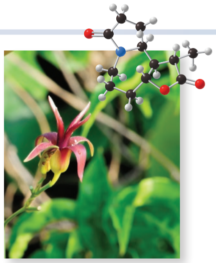

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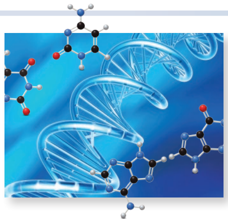

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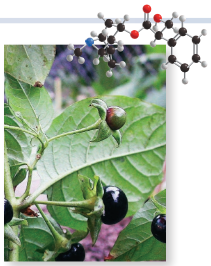

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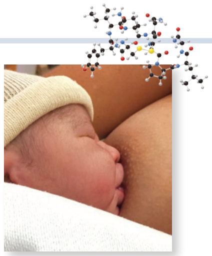

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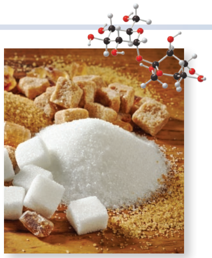

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Preface

Since the publication of *Organic Chemistry* in 2005, chemistry has witnessed a rapid growth in its understanding of the biological world. The molecular basis of many complex biological processes is now known with certainty, and can be explained by applying the basic principles of organic chemistry. Because of the close relationship between chemistry and many biological phenomena, *Organic Chemistry with Biological Topics* presents an approach to traditional organic chemistry that incorporates the discussion of biological applications that are understood using the fundamentals of organic chemistry.

The Basic Features

Organic Chemistry with Biological Topics continues the successful student-oriented approach used in *Organic Chemistry* by Janice Gorzynski Smith. This text uses less prose and more diagrams and bulleted summaries for today's students, who rely more heavily on visual imagery to learn than ever before. Each topic is broken down into small chunks of information that are more manageable and easily learned. Sample Problems illustrate stepwise problem solving, and relevant examples from everyday life are used to illustrate topics. New concepts are introduced one at a time so that the basic themes are kept in focus.

The organization of *Organic Chemistry with Biological Topics* provides the student with a logical and accessible approach to an intense and fascinating subject. The text begins with a healthy dose of review material in Chapters 1 and 2 to ensure that students have a firm grasp of the fundamentals. Stereochemistry, the three-dimensional structure of molecules, is introduced early (Chapter 5) and reinforced often. Certain reaction types with unique characteristics and terminology are grouped together. These include acid–base reactions (Chapter 2), oxidation and reduction (Chapters 11 and 13), reactions of organometallic reagents (Chapter 13), and radical reactions (Chapter 21). Because of its importance in biological molecules, **the chemistry of carbonyl-containing compounds has been moved much earlier** than traditional organic chemistry texts and is now described in Chapters 13–18. Each chapter ends with a Chapter Review, end-of-chapter summaries that succinctly organize the main concepts and reactions.

New to This Edition

Students sometimes ask me if the facts of organic chemistry have significantly changed since the last edition. While the basic principles remain the same—carbon forms four bonds in stable compounds and oppositely charged species attract each other—organic chemistry is a dynamic subject that is continually refined as new facts are determined, and new editions reflect current understanding. Each year, novel compounds are discovered and new drugs are marketed, and these compounds replace older examples to illustrate particular concepts. Also of significance is *how* the material in the text is presented. I continue to endeavor to make this difficult subject as student-friendly as possible, by redesigning sample problems and end-of-chapter material, and rewriting sentences and paragraphs for improved clarity.

General

Expanded Problem-Solving Approach A central component of each chapter of *Organic Chemistry with Biological Topics* is the Sample Problems, which illustrate how to solve key elements of the chapter. In this edition, Sample Problems are always paired with a follow-up Problem to allow students to apply what they have just learned. The Problems are followed by "More Practice," a list of end-of-chapter problems that are similar in concept. Students can find detailed solutions and verify their answers to *all* of the Problems from the book with the Student Study Guide/Solutions Manual for *Organic Chemistry with Biological Topics*.

Chapter Review The end-of-chapter summary sections have been expanded into parts: **Key Concepts, Key Skills, Key Reactions,** and **Key Mechanism Concepts,** with structures and examples to illustrate each part, providing students with a broader and more detailed overview of each chapter's important concepts and skills. Extensive cross-referencing has also been added to connect this material with relevant Sample Problems, Problems, Figures, and Tables within the body of the chapter.

New Chapters

In addition to the six chapters that contained new biological material in the fifth edition—Chapters 3, 6, 15, 16, 18, and 19—two new chapters have been added:

- **Chapter 26** provides an in-depth discussion of the structure and properties of the nucleic acids DNA and RNA. Three key processes are also presented: replication—how DNA makes copies of itself; transcription—how the genetic information in DNA is passed onto RNA; and translation—how the coded genetic information in RNA is used to synthesize proteins. The chapter concludes with discussions of manipulating DNA in the laboratory and how viruses act.
- **Chapter 27** focuses on the biochemical reactions involved in metabolism. The discussion centers on three components: the breakdown of fats, the metabolism of the carbohydrate glucose to the three-carbon unit pyruvate by glycolysis, and the citric acid cycle, a key cyclic metabolic pathway used for amino acids, carbohydrates, and fats.

Spectroscopy

The revisions to the spectroscopy coverage are designed to allow for more flexibility, making these chapters more portable to accommodate various lecture and lab arrangements. Three new spectroscopy chapters have been created for the sixth edition: Spectroscopy A Mass Spectrometry; Spectroscopy B Infrared Spectroscopy; and Spectroscopy C Nuclear Magnetic Resonance Spectroscopy. The coverage and problem sets for these chapters have also been expanded to include material previously covered in other sections of earlier editions. Extensive cross-referencing has been added so that whether spectroscopy is covered early or late in an organic chemistry course, students can readily find the material they need.

Other New Coverage

Examples of biomolecules are sprinkled throughout the chapters to illustrate common organic structural features and reactions, such as Lewis structures (Chapter 1), Lewis acids and bases (Chapter 2), stereochemistry (Chapter 5), and elimination reactions (Chapters 8 and 9). Other changes include the following:

- Section 11.13 on biological oxidation has been expanded to include the treatment of prochirality.
- New material has been added to Sections 13.6 and 13.7, including the biological reduction of acyl phosphates to aldehydes.
- The role of imines in the deamination of amino acids is discussed in Section 14.13B, and a detailed mechanism that illustrates the role of pyridoxal phosphate, vitamin B_6, is presented.
- The coverage of nitriles has been moved to the chapter on carboxylic acids, forming Chapter 15, Carboxylic Acids and Nitriles. This chapter is now placed after Chapter 14, Aldehydes and Ketones, and this move offers two advantages. The chapter places the chemistry of carboxylic acids closer to similar chemistry seen with the acyl derivatives that is covered in Chapter 16. It also places the nucleophilic addition reactions of nitriles in closer proximity to related reactions in Chapter 14.
- A new Section 17.11 on biological decarboxylation has been added to Chapter 17.
- A new Section 23.8D on protein denaturation has been added to Chapter 23.
- Section 23.10 on enzymes illustrates how enzymes work with a specific example, how the serine proteases hydrolyze peptide bonds in proteins. The section concludes with a discussion of how enzymes are used to diagnose and treat diseases.
- The importance of human milk oligosaccharides in breast milk is discussed in Section 24.12D.

Learning Resources for Instructors and Students

The following items may accompany this text. Please consult your McGraw-Hill representative for policies, prices, and availability as some restrictions may apply.

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Within the Instructor's Resources, instructors have access to editable, accessible PowerPoint lecture outlines, which appear as ready-made presentations that combine art and lecture notes for each chapter of the text. For instructors who prefer to create their lecture notes from scratch, all illustrations, photos, tables, *How To*'s, and Sample Problems are pre-inserted by chapter into a separate set of PowerPoint slides. They are also available as individual .jpg files.

Photos, artwork, and other media types can be used to create customized lectures, visually enhanced tests and quizzes, compelling course websites, or attractive printed support materials. All assets are copyrighted by McGraw-Hill Higher Education, but can be used by instructors for classroom purposes. The visual resources in this collection include:

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- **Photos** The photo collection contains digital files of photographs from the text, which can be reproduced for multiple classroom uses.
- **Tables** Every table that appears in the text has been saved in electronic form for use in classroom presentations and/or quizzes.

Student Study Guide/Solutions Manual

Written by Janice Gorzynski Smith and Erin R. Smith, the Student Study Guide/Solutions Manual provides step-by-step solutions to all in-chapter and end-of-chapter problems. Each chapter begins with an overview of key concepts and includes a short-answer practice test on the fundamental principles and new reactions.

Acknowledgments

Although I have been an author for many years, this edition of *Organic Chemistry with Biological Topics* reflects recent advances in our understanding of organic chemistry, as well as new advances in digital media that allow this work to be better understood by a larger student audience. To produce a high quality text and ancillary materials requires not only my insights as an author, but also the expertise of a group of individuals with whom I work, beginning with the generation of a manuscript, progressing through the publication of the finished product both in print and digital form, and bringing the text to the larger chemistry community by the sales and marketing team.

My special thanks in this edition go out to two individuals who are integral to success of the project. Mary Hurley, Senior Developmental Editor, with whom I have worked for several years, is a master at supervising all the details of this large project and heading off problems before they become crises. I feel that Mary has been key in keeping my projects on a smooth trajectory even when many of the other personnel involved have changed. Amy Gehl, Production Manager, although new to the team, has skillfully and seamlessly managed the conversion of this text from paper manuscript to printed edition. Thanks so much to both of you and my sincere appreciation goes out to the entire chemistry group.

I especially thank my husband Dan and the other members of my immediate family, who have experienced the day-to-day demands of living with a busy author. The joys and responsibilities of the family have always kept me grounded during the rewarding but sometimes all-consuming process of writing a textbook. This book, like the prior edition of *Organic Chemistry with Biological Topics,* is dedicated to my wonderful daughter Megan, who passed away after a nine-year battle with cystic fibrosis.

Among the many others that go unnamed but who have profoundly affected this work are the thousands of students I have been lucky to teach over many years. I have learned so much from my daily interactions with them, and I hope that the wider chemistry community can benefit from this experience.

This edition has evolved based on the helpful feedback of many people who reviewed past editions and digital products, class-tested the book, and attended focus groups or symposiums. These many individuals have collectively provided constructive improvements to the project.

Listed below are the reviewers of *Organic Chemistry with Biological Topics,* fifth edition:

Steven Castle, *Brigham Young University*
Manashi Chatterjee, *Hunter College*
Emma Chow, *Palm Beach State College*
Jeff Corkill, *Eastern Washington University*
Andrew Frazer, *University of Central Florida*
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Lisa Whalen, *University of New Mexico*
Alexander Wurthmann, *University of Vermont*

The following individuals helped write and review learning goal-oriented content for **SmartBook for Organic Chemistry with Biological Topics:** David Jones, St. David's School in Raleigh, NC; Adam Keller, Columbus State Community College; and Angela Perkins, University of Minnesota. Andrea Leonard of the University of Louisiana, Lafayette, revised the PowerPoint Lectures, and Ryan Simon also of the University of Louisiana, Lafayette, revised the Test Bank for *Organic Chemistry with Biological Topics*, sixth edition.

Although every effort has been made to make this text and its accompanying Student Study Guide/Solutions Manual as error-free as possible, some errors undoubtedly remain. Please feel free to email me about any inaccuracies, so that subsequent editions may be further improved.

With much aloha,

Janice Gorzynski Smith
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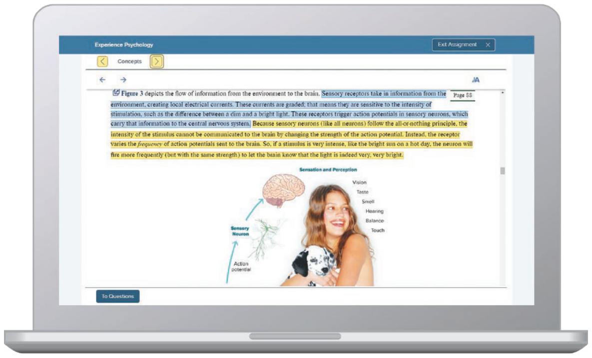

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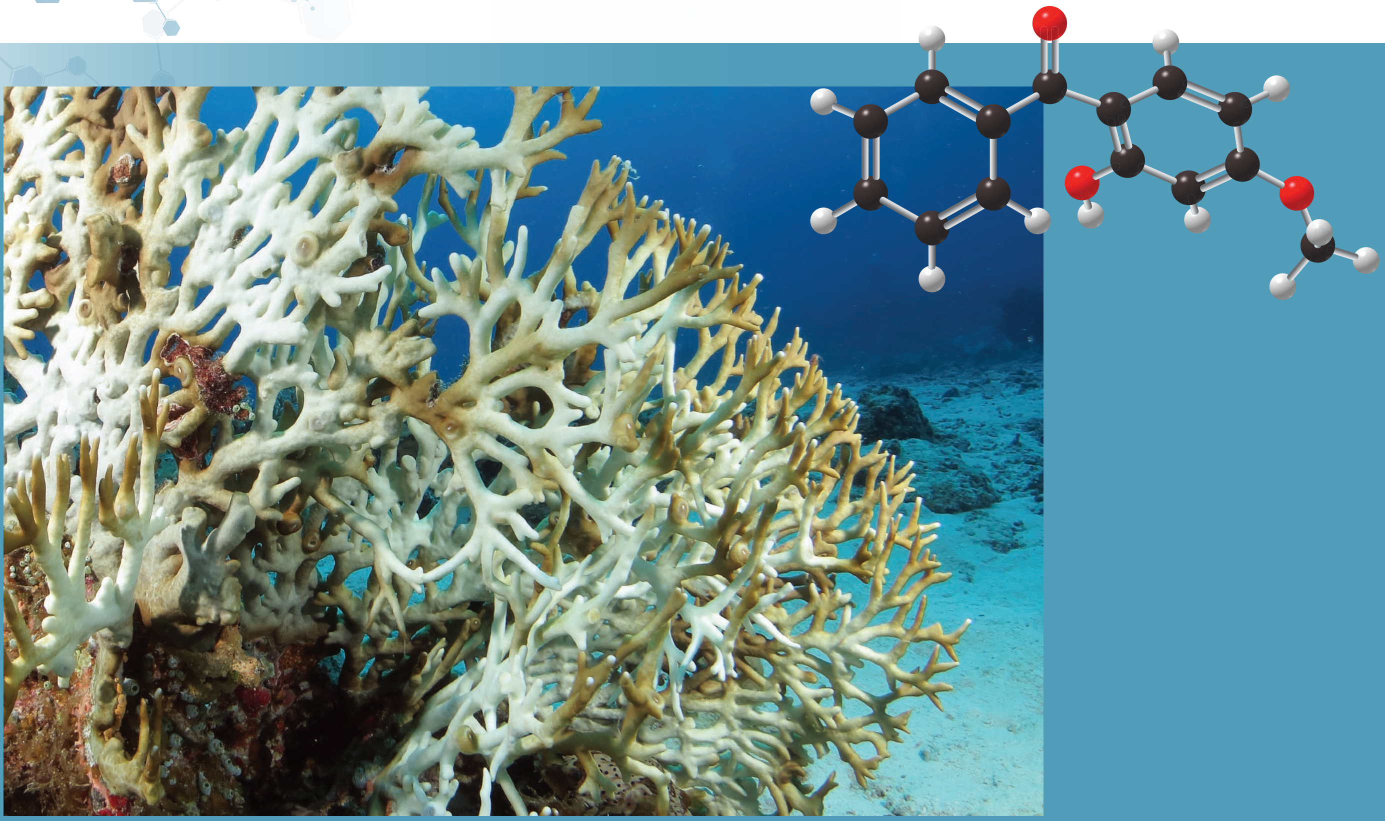
1

Structure and Bonding



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Bleaching is a phenomenon that occurs when corals expel symbiotic algae from their tissues in response to an external stress, causing the coral to turn white. Although coral bleaching is most often associated with an increase in water temperature, recent research at the University of Hawai‘i suggests that minute amounts of compounds such as **oxybenzone** also contribute to bleaching. Oxybenzone effectively filters a broad spectrum of harmful ultraviolet light, so it is a common sunscreen component, but it can be washed off while swimming, leading to a low but potentially harmful concentration in the water. For this reason, the state of Hawai‘i now prohibits the sale of sunscreens that contain oxybenzone. In Chapter 1, we learn about the structure, bonding, and properties of organic compounds like oxybenzone.

Why Study . . .

Structure and Bonding?

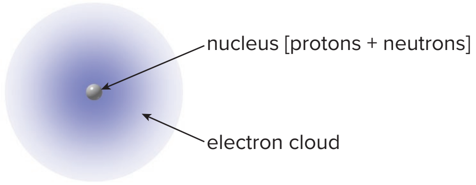
Before examining organic molecules in detail, we must review topics about structure and bonding learned in previous chemistry courses. We will discuss these concepts primarily from an organic chemist's perspective, and spend time on only the particulars needed to understand organic compounds.

Important topics in Chapter 1 include drawing Lewis structures, predicting the shape of molecules, determining what orbitals are used to form bonds, and how electronegativity affects bond polarity. Equally important is Section 1.8 on drawing organic molecules, both shorthand methods routinely used for simple and complex compounds, and three-dimensional representations that allow us to more clearly visualize them.

1.1 The Periodic Table

All matter is composed of the same building blocks called **atoms.** There are two main components of an atom.

- The **nucleus** contains positively charged **protons** and uncharged **neutrons. Most of the mass of the atom is contained in the nucleus.**
- The **electron cloud** is composed of negatively charged **electrons. The electron cloud comprises most of the volume of the atom.**



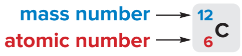
The charge on a proton is equal in magnitude but opposite in sign to the charge on an electron. In a neutral atom, the **number of protons in the nucleus equals the number of electrons.** This quantity, called the **atomic number,** is unique to a particular element. For example, every neutral carbon atom has an atomic number of six, meaning it has six protons in its nucleus and six electrons surrounding the nucleus.

In addition to neutral atoms, we will encounter **charged ions.**

- A *cation* is positively charged and has fewer electrons than protons.
- An *anion* is negatively charged and has more electrons than protons.

The number of neutrons in the nucleus of a particular element can vary. **Isotopes** are two atoms of the same element having a different number of neutrons. The **mass number** of an atom is the total number of protons and neutrons in the nucleus. **Isotopes have *different* mass numbers.** The **atomic weight** of a particular element is the weighted average of the mass of all its isotopes, reported in atomic mass units (amu).

Isotopes of carbon and hydrogen are sometimes used in organic chemistry. The most common isotope of hydrogen has one proton and no neutrons in the nucleus, but 0.02% of hydrogen atoms have one proton and one neutron. This isotope of hydrogen is called **deuterium** and is sometimes symbolized by the letter **D.**



Each atom is identified by a one- or two-letter abbreviation that is the characteristic symbol for that element. Carbon is identified by the single letter **C.** Sometimes the atomic number is indicated as a subscript to the left of the element symbol, and the mass number is indicated as a superscript. Using this convention, the most common isotope of carbon, which contains six protons and six neutrons, is designated as **${}^{12}_{6}\mathrm{C}$.**

A **row** in the periodic table is also called a ***period,*** and a **column** is also called a ***group.*** A periodic table is located in Appendix A for your reference.

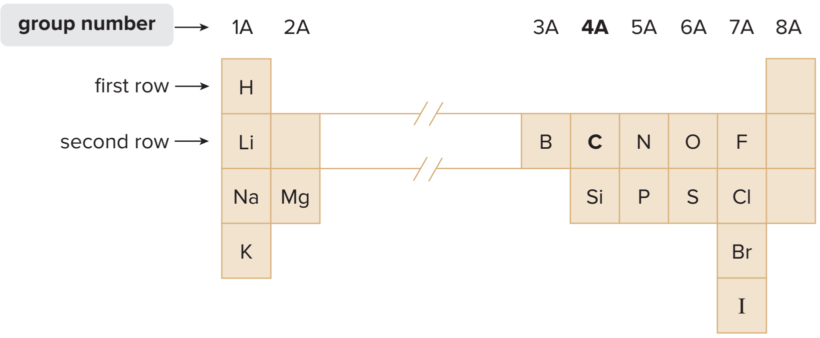
The **periodic table** is a schematic arrangement of the more than 100 known elements, arranged in order of increasing atomic number. The periodic table is composed of rows and columns. Each column in the periodic table is identified by a **group number,** an Arabic (1 to 8) or Roman (I to VIII) numeral followed by the letter A or B. Carbon is located in group **4A** in the periodic table in this text.

- Elements in the same row are similar in *size.*
- Elements in the same column have similar *electronic and chemical properties.*

Although more than 100 elements exist, most are not common in organic compounds. Figure 1.1 contains a truncated periodic table, indicating the handful of elements that are routinely seen in this text. **Most elements in organic compounds are located in the first and second rows of the periodic table.**

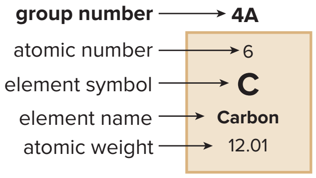
Figure 1.1

A periodic table of the common elements seen in organic chemistry



- Carbon is located in the second row, group **4A.**

Carbon's entry in the periodic table:

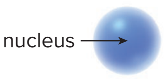


Across each row of the periodic table, electrons are added to a particular shell of orbitals around the nucleus. Adding electrons to the first shell forms the first row. Adding electrons to the second shell forms the second row. **Electrons are first added to the shells closest to the nucleus.**

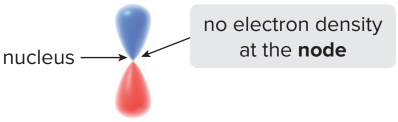
Each shell contains a certain number of **orbitals.** An orbital is a region of space that is high in electron density. There are four different kinds of orbitals, called ***s, p, d,*** and ***f.*** The first shell has only one orbital, an *s* orbital. The second shell has two kinds of orbitals, *s* and ***p,*** and so on. Each type of orbital has a particular shape.

For the first- and second-row elements, we must consider only ***s* orbitals** and ***p* orbitals.**

- An ***s* orbital** has a **sphere of electron density.** It is ***lower in energy*** than other orbitals of the same shell, because electrons are kept closer to the positively charged nucleus.
- A ***p* orbital** has a **dumbbell shape.** It contains a **node of electron density** at the nucleus. A node means there is *no* electron density in this region. A *p* orbital is ***higher in energy*** than an *s* orbital (in the same shell) because its electron density is farther away from the nucleus.



***s* orbital**
lower in energy



***p* orbital**
higher in energy

An *s* orbital is filled with electrons before a *p* orbital in the same shell.

1.1A The First Row

The first row of the periodic table is formed by adding electrons to the only orbital in the first shell, called the **1*s* orbital.**

- Each orbital can have a maximum of two electrons.

H

$1s^1$

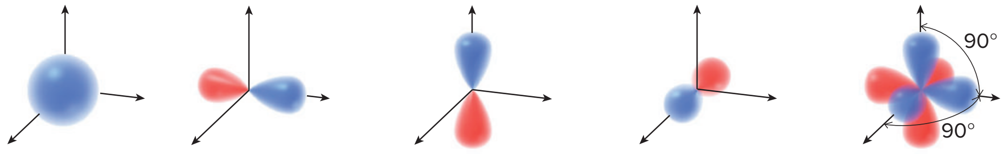
one electron in the 1*s* orbital

As a result, there are **two elements in the first row,** one having one electron added to the 1*s* orbital and one having two. The element **hydrogen (H)** has what is called a $1s^1$ configuration with one electron in the 1*s* orbital, and **helium (He)** has a $1s^2$ configuration with two electrons in the 1*s* orbital.

1.1B The Second Row

Every element in the second row has a filled first shell of electrons. Thus, all second-row elements have a $1s^2$ configuration. Each element in the second row of the periodic table also has four orbitals available to accept additional electrons:

- **one 2*s* orbital,** the *s* orbital in the second shell
- **three 2*p* orbitals,** all dumbbell-shaped and perpendicular to each other along the *x, y,* and *z* axes



2*s* orbital

$2p_x$ orbital

$2p_y$ orbital

$2p_z$ orbital

all three 2*p* orbitals drawn on the same set of axes

Because each of the four orbitals in the second shell can hold two electrons, there is a **maximum capacity of *eight* electrons** for elements in the second row. The second row of the periodic table consists of eight elements, obtained by adding electrons to the 2*s* and three 2*p* orbitals.

group number	1A	2A	3A	**4A**	5A	6A	7A	8A
second row	Li	Be	B	**C**	N	O	F	Ne
number of **valence electrons**	1	2	3	**4**	5	6	7	8

The outermost electrons are called **valence electrons.** The valence electrons are more loosely held than the electrons closer to the nucleus, and as such, they participate in chemical reactions. **The group number of a second-row element reveals its number of valence electrons.** For example, carbon in group 4A has four valence electrons, and oxygen in group 6A has **six.**

Problem 1.1 While the most common isotope of nitrogen has a mass number of 14 (nitrogen-14), a radioactive isotope of nitrogen has a mass number of 13 (nitrogen-13). Nitrogen-13 is used in PET (positron emission tomography) scans by physicians to monitor brain activity and diagnose dementia. For each isotope, give the following information: (a) the number of protons; (b) the number of neutrons; (c) the number of electrons in the neutral atom; (d) the group number; and (e) the number of valence electrons.

1.2 Bonding

Until now our discussion has centered on individual atoms, but it is more common in nature to find two or more atoms joined together.

- ***Bonding*** **is the joining of two atoms in a stable arrangement.**

Joining two or more elements forms **compounds.** Examples of compounds include hydrogen gas (H_2), formed by joining two hydrogen atoms, and methane (CH_4), the simplest organic compound, formed by joining a carbon atom with four hydrogen atoms.

One general rule governs the bonding process.

- Through bonding, atoms attain a complete outer shell of valence electrons.

Because the noble gases in group 8A of the periodic table are especially stable as atoms having a filled shell of valence electrons, the general rule can be restated.

- Through bonding, atoms gain, lose, or share electrons to attain the electronic configuration of the noble gas closest to them in the periodic table.

Atoms readily form ionic bonds when they can attain a noble gas configuration by gaining or losing just one or two electrons. NaCl and KI are ionic compounds. *Jill Braaten*

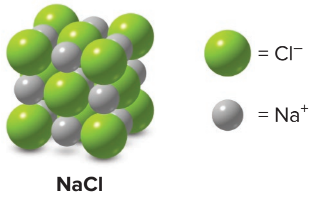
What does this mean for first- and second-row elements? **A first-row element like hydrogen can accommodate *two electrons* around it.** This would make it like the noble gas helium at the end of the same row. **A second-row element is generally most stable with *eight valence electrons* around it** like neon. Elements that behave in this manner are said to follow the **octet rule.**

There are two different kinds of bonding: **ionic bonding** and **covalent bonding.**

- *Ionic bonds* result from the *transfer* of electrons from one element to another.
- *Covalent bonds* result from the *sharing* of electrons between two nuclei.

The type of bonding is determined by the location of an element in the periodic table. An **ionic bond** generally occurs when elements on the **far left** side of the periodic table combine with elements on the **far right** side, ignoring the noble gases, which form bonds only rarely. **The resulting ions are held together by extremely strong electrostatic interactions.** A positively charged **cation** formed from the element on the left side attracts a negatively charged **anion** formed from the element on the right side. Examples of ionic inorganic compounds include sodium chloride (NaCl), common table salt, and potassium iodide (KI), an essential nutrient added to make iodized salt.

Ionic compounds form extended crystal lattices that maximize the positive and negative electrostatic interactions. In NaCl, each positively charged Na^+ ion is surrounded by six negatively charged Cl^- ions, and each Cl^- ion is surrounded by six Na^+ ions.



- The transfer of electrons forms stable salts composed of cations and anions.

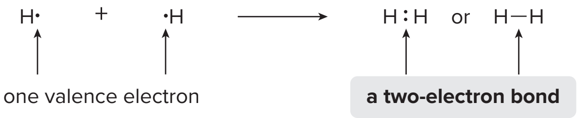
A **compound** may have either ionic or covalent bonds. A **molecule** has only covalent bonds.

The second type of bonding, **covalent bonding,** occurs with elements like carbon in the middle of the periodic table, which would otherwise have to gain or lose several electrons to form an ion with a complete valence shell. **A covalent bond is a two-electron bond,** and a compound with covalent bonds is called a **molecule.** Covalent bonds also form between two elements from the same side of the table, such as two hydrogen atoms or two chlorine atoms. H_2, Cl_2, and CH_4 are all examples of covalent molecules.

Problem 1.2 Label each bond in the following compounds as ionic or covalent.

a. F_2 b. LiBr c. CH_3CH_3 d. $NaNH_2$ e. $NaOCH_3$

How many covalent bonds will a particular atom typically form? As you might expect, it depends on the location of the atom in the periodic table. In the first row, **hydrogen forms one covalent bond** using its one valence electron. When two hydrogen atoms are joined in a bond, each has a filled valence shell of two electrons. **A *solid line* indicates a two-electron bond.**



Second-row elements can have no more than eight valence electrons around them. For neutral molecules, two consequences result.

- **Atoms with one, two, three, or four valence electrons form one, two, three, or four bonds,** respectively, in neutral molecules.
- **Atoms with five or more valence electrons** form enough bonds to give an octet. In this case, **the predicted number of bonds = 8 – the number of valence electrons.**

For example, B has three valence electrons, so it forms three bonds, as in BF_3. N has five valence electrons, so it also forms three bonds (8 – 5 = 3 bonds), as in NH_3.

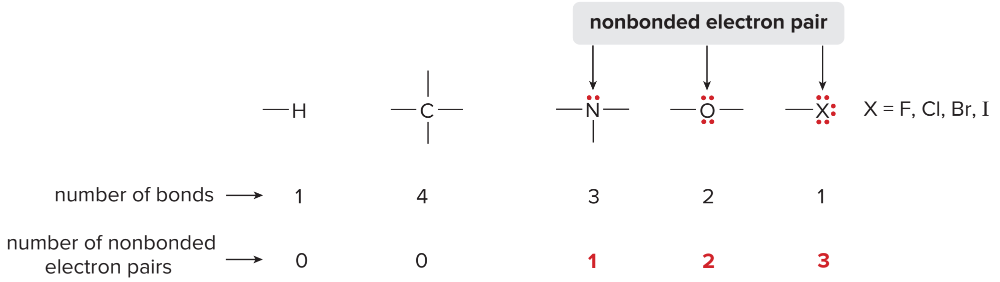
Nonbonded pair of electrons = unshared pair of electrons = lone pair

These guidelines are used in Figure 1.2 to summarize the usual number of bonds formed by the common atoms in organic compounds. When second-row elements form fewer than four bonds, their octets consist of both **bonding (shared) electrons** and **nonbonding (unshared) electrons.** Unshared electrons are also called **lone pairs.**

Problem 1.3 How many covalent bonds are predicted for each atom?

a. O b. Al c. Br d. Si

Figure 1.2 The usual number of bonds of common neutral atoms



1.3 Lewis Structures

***Lewis structures* are electron dot representations for molecules.** Three rules are used for drawing Lewis structures.

1. Draw only the valence electrons.
2. Give every second-row element no more than *eight* electrons.
3. Give each hydrogen *two* electrons.

1.3A A Procedure for Drawing Lewis Structures

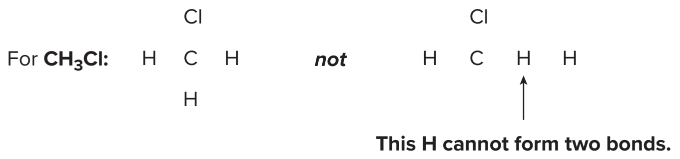
Follow a stepwise procedure to draw a Lewis structure.

How To Draw a Lewis Structure

Step [1] **Arrange atoms next to each other that you think are bonded together.**

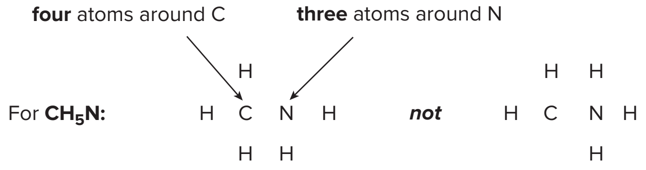
- Always place hydrogen atoms and halogen atoms on the periphery because H and X (X = F, Cl, Br, and I) form only one bond each.

The letter **X** is often used to represent one of the halogens in group 7A: F, Cl, Br, or I.



—*Continued*

- As a first approximation, use the common bonding patterns in Figure 1.2 to arrange the atoms.



- In truth, the proper arrangement of atoms may not be obvious, or more than one arrangement may be possible (Section 1.4). Even in many simple molecules, the connectivity between atoms must be determined experimentally.

Step [2] **Count the electrons.**

- Count the number of valence electrons from all atoms.
- **Add one electron** for each *negative* charge.
- **Subtract one electron** for each *positive* charge.
- This sum gives the total number of electrons that must be used in drawing the Lewis structure.

Step [3] **Arrange the electrons around the atoms.**

- Place a bond between every two atoms, giving **two electrons to each H** and **no more than eight to any second-row atom.**
- Use all remaining electrons to **fill octets with lone pairs.**
- If all valence electrons are used and an atom does not have an octet, form multiple bonds, as shown in Sample Problem 1.2.

Step [4] **Assign formal charges to all atoms.**

- Formal charges are discussed in Section 1.3C.

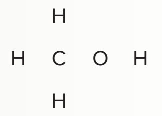
Sample Problem 1.1 illustrates how to draw the Lewis structure of a simple organic molecule.

Sample Problem 1.1 Drawing a Lewis Structure for a Simple Molecule

Draw a Lewis structure for methanol, a compound with molecular formula CH_4O.

Solution

Step [1] **Arrange the atoms.**



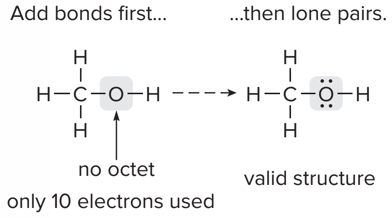
- Place the second-row elements, C and O, in the middle.
- Place three H's around C to surround C by four atoms.
- Place one H next to O to surround O by two atoms.

Step [2] **Count the electrons.**

$$\begin{aligned} 1\,C \times 4\,e^- &= 4\,e^- \\ 1\,O \times 6\,e^- &= 6\,e^- \\ 4\,H \times 1\,e^- &= \underline{4\,e^-} \\ & \mathbf{14\ e^-\ total} \end{aligned}$$

Step [3] **Add the bonds and lone pairs.**

- Add five two-electron bonds to form the C–H, C–O, and O–H bonds, using 10 of the 14 electrons.
- Place two lone pairs on the O atom to use the remaining four electrons and give the O atom an octet.



This Lewis structure is valid because it uses all 14 electrons, each H is surrounded by two electrons, and each second-row element is surrounded by no more than eight electrons.

Problem 1.4 Draw a valid Lewis structure for each species.

a. CH_3CH_3 b. CH_5N c. C_2H_5Br

More Practice: Try Problem 1.45a.

1.3B Multiple Bonds

Sample Problem 1.2 illustrates an example of a Lewis structure with a double bond.

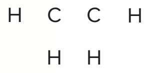
Sample Problem 1.2 Drawing a Lewis Structure with a Multiple Bond

Draw a Lewis structure for ethylene, a compound of molecular formula C_2H_4, in which each carbon is bonded to two hydrogens.

Solution

Follow Steps [1] to [3] to draw a Lewis structure.

Step [1] **Arrange the atoms.**

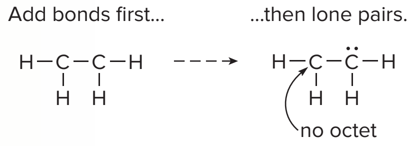


- Each C gets 2 H's.

Step [2] **Count the electrons.**

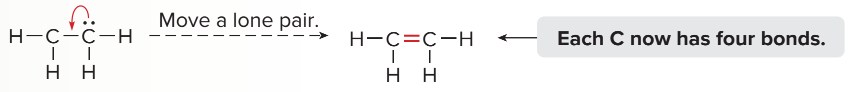
$$\begin{array}{rcl} 2\ C \times 4\ e^- & = & 8\ e^- \\ 4\ H \times 1\ e^- & = & \underline{4\ e^-} \\ & & \mathbf{12\ e^-\ total} \end{array}$$

Step [3] **Add the bonds and lone pairs.**



After placing five bonds between the atoms and adding the two remaining electrons as a lone pair, one C still has no octet.

To give both C's an octet, **change *one* lone pair into *one* bonding pair of electrons between the two C's, forming a double bond.**

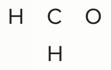


ethylene
a valid Lewis structure

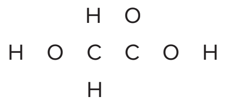
This uses all 12 electrons, each C has an octet, and each H has two electrons. The Lewis structure is valid. **Ethylene contains a carbon–carbon double bond.**

Problem 1.5 Draw an acceptable Lewis structure for each compound, assuming the atoms are connected as arranged. Formaldehyde (H_2CO) is a preservative, and glycolic acid ($HOCH_2CO_2H$) is used to make dissolving sutures.

a. H_2CO



b. $HOCH_2CO_2H$

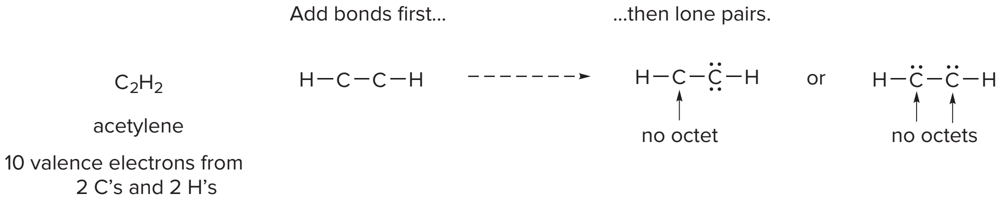


More Practice: Try Problems 1.44, 1.45b–d.

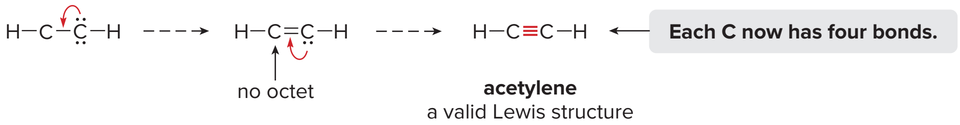
- After placing all electrons in bonds and lone pairs, use a lone pair to form a multiple bond if an atom does not have an octet.

Carbon always forms four bonds in stable organic molecules. Carbon forms single, double, and triple bonds to itself and other elements.

You must change *one* lone pair into *one* new bond for each *two* electrons needed to complete an octet. In acetylene, a compound with molecular formula C_2H_2, placing the 10 valence electrons gives a Lewis structure in which one or both of the C's lack an octet.



In this case, **change *two* lone pairs into *two* bonding pairs of electrons, forming a triple bond.**



Problem 1.6 Draw an acceptable Lewis structure for each compound, assuming the atoms are connected as arranged.

a. HCN H C N

b. C_3H_4

H
H C C C H
H

1.3C Formal Charge

To manage electron bookkeeping in a Lewis structure, chemists use **formal charge.**

- *Formal charge* is the charge assigned to individual atoms in a Lewis structure.

By calculating formal charge, we determine how the number of electrons around a particular atom compares to its number of valence electrons. Formal charge is calculated as follows:

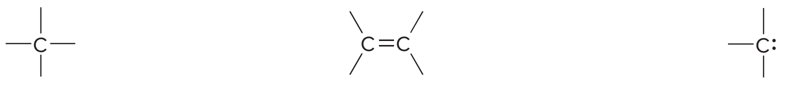
$$\text{formal charge} = \text{number of valence electrons} - \text{number of electrons an atom “owns”}$$

The number of electrons “owned” by an atom is determined by its number of bonds and lone pairs.

- An atom “owns” *all* of its unshared electrons and *half* of its shared electrons.

$$\text{number of electrons owned} = \text{number of unshared electrons} + \frac{1}{2}\left[\text{number of shared electrons}\right]$$

The number of electrons “owned” by different carbon atoms is indicated in the following examples:



- C shares eight electrons.
- C “owns” **four** electrons.

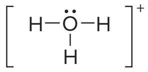
- Each C shares eight electrons.
- Each C “owns” **four** electrons.

- C shares six electrons.
- C has two unshared electrons.
- C “owns” **five** electrons.

Sample Problem 1.3 illustrates how formal charge is calculated on the atoms of a polyatomic ion. **The sum of the formal charges on the individual atoms equals the net charge on the molecule or ion.**

Sample Problem 1.3 Determining the Formal Charge on an Atom

Determine the formal charge on each atom in the ion H_3O^+.

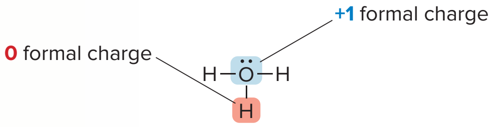


$[H-\ddot{O}(-H)-H]^+$

Solution

To calculate the formal charge on each atom:

- **Determine the number of valence electrons from the group number.**
- **Determine the number of electrons an atom "owns"** from the number of bonding and nonbonding electrons it has.
- **Subtract** the second quantity from the first to give the formal charge.



For the O atom (group **6**A):

- number of valence electrons = **6**
- number of bonding electrons = 6
- number of nonbonding electrons = 2

$$\text{formal charge} = 6 - \left[2 + \frac{1}{2}(6)\right] = +1$$

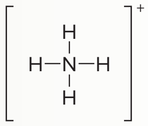
For each H atom (group **1**A):

- number of valence electrons = **1**
- number of bonding electrons = 2
- number of nonbonding electrons = 0

$$\text{formal charge} = 1 - \left[0 + \frac{1}{2}(2)\right] = 0$$

The formal charge on the O atom is **+1** and the formal charge on each H is **0.** The overall charge on the ion H_3O^+ is the sum of all of the formal charges on the atoms: 1 + 0 + 0 + 0 = +1.

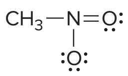
Problem 1.7 Calculate the formal charge on each second-row atom.

a. 

$[NH_4]^+$

b. $CH_3-N\equiv C:$

c. $:\ddot{O}=\ddot{O}-\underset{\cdot\cdot}{\ddot{O}}:$

d. 

$CH_3-N=\ddot{O}:$ with $:\ddot{O}:$ on N

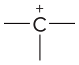
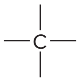
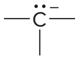
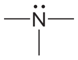
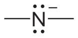
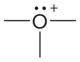
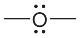
More Practice: Try Problems 1.42, 1.43.

Problem 1.8 Draw a Lewis structure for each ion.

a. CH_3O^- b. HC_2^- c. $(CH_3NH_3)^+$ d. $(CH_3NH)^-$

When you first add formal charges to Lewis structures, use the procedure in Sample Problem 1.3. With practice, you will notice that certain bonding patterns always result in the same formal charge. For example, any N atom with four bonds (and thus no lone pairs) has a +1 formal charge. Table 1.1 lists the bonding patterns and resulting formal charges for carbon, nitrogen, and oxygen.

Table 1.1 Formal Charge Observed with Common Bonding Patterns for C, N, and O

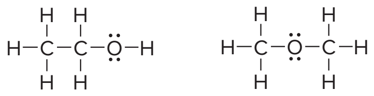
Atom	Number of valence electrons	Formal charge		
		+1	0	–1
C	4			
N	5			
O	6			

Problem 1.9 What is the formal charge on the O atom in each of the following species that contains a multiple bond to O?

a. ≡O: b. =O̤— c. =O̤:

1.4 Isomers

Sometimes in drawing a Lewis structure, more than one arrangement of atoms is possible for a given molecular formula. For example, there are two acceptable arrangements of atoms for the molecular formula C_2H_6O.



ethanol dimethyl ether

same molecular formula
C_2H_6O
isomers

Both are valid Lewis structures, and both molecules exist. One is called ethanol, and the other, dimethyl ether. These two compounds are called **isomers.**

- *Isomers* are different molecules having the same molecular formula.

Ethanol and dimethyl ether are **constitutional isomers** because they have the same molecular formula, but the ***connectivity of their atoms is different.*** Ethanol has one C–C bond and one O–H bond, whereas dimethyl ether has two C–O bonds. A second class of isomers, called **stereoisomers,** is introduced in Section 4.13B.

Problem 1.10 Draw Lewis structures for each molecular formula.

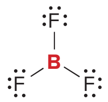
a. $C_2H_4Cl_2$ (two isomers) b. C_3H_8O (three isomers) c. C_3H_6 (two isomers)

1.5 Exceptions to the Octet Rule

Most of the common elements in organic compounds—**C, N, O, and the halogens**—follow the octet rule. **Hydrogen** is a notable exception, because it accommodates only two electrons in bonding. Additional exceptions include **boron** and **beryllium** (second-row elements in groups 3A and 2A, respectively), and elements in the third row (particularly **phosphorus** and **sulfur**).

Elements in groups 2A and 3A of the periodic table, such as beryllium and boron, do not have enough valence electrons to form an octet in a neutral molecule. Lewis structures for BeH_2 and BF_3 show that these atoms have only four and six electrons, respectively, around the central atom. There simply aren't enough electrons to form an octet. Because the Be and B atoms each have less than an octet of electrons, these molecules are highly reactive.

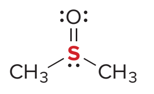
four electrons around Be



six electrons around B

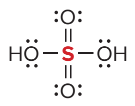
A second exception to the octet rule occurs with some elements located in the third row and later in the periodic table. These elements have empty *d* orbitals available to accept electrons, and thus they may have ***more than eight*** **electrons** around them. For organic chemists, the two most common elements in this category are **phosphorus** and **sulfur,** which can have 10 or even 12 electrons around them, as shown in dimethyl sulfoxide (a common solvent), sulfuric acid (a strong inorganic acid), and glyceraldehyde 3-phosphate (an intermediate formed during carbohydrate metabolism).

10 electrons around S



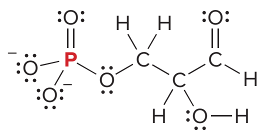
dimethyl sulfoxide
DMSO

12 electrons around S



sulfuric acid

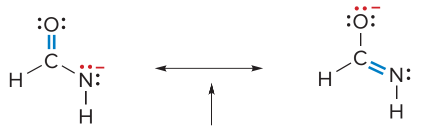
10 electrons around P



glyceraldehyde 3-phosphate

1.6 Resonance

Some molecules can't be adequately represented by a single Lewis structure. For example, two valid Lewis structures can be drawn for the anion $(HCONH)^-$. One structure has a negatively charged N atom and a C–O double bond; the other has a negatively charged O atom and a C–N double bond. These structures are called **resonance structures** or **resonance forms.** A **double-headed arrow** is used to separate two resonance structures.



double-headed arrow

- *Resonance structures* are two Lewis structures having the *same* placement of atoms but a *different* arrangement of electrons.

Which resonance structure is an accurate representation for $(HCONH)^-$? **The answer is *neither* of them.** The true structure is a composite of both resonance forms, and is called a **resonance hybrid.** The hybrid shows characteristics of ***both*** resonance structures.

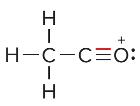
Each resonance structure implies that electron pairs are localized in bonds or on atoms. In actuality, resonance allows certain electron pairs to be ***delocalized*** over two or more atoms, and this delocalization of electron density adds stability. **A molecule with two or more resonance structures is said to be *resonance stabilized.***

1.6A An Introduction to Resonance Theory

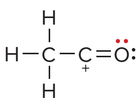
Keep in mind the following basic principles of resonance theory.

- Resonance structures are *not* real. An individual resonance structure does not accurately represent the structure of a molecule or ion.
- Resonance structures are *not* in equilibrium with each other. There is no movement of electrons from one form to another.
- Resonance structures are *not* isomers. Two isomers differ in the arrangement of *both* atoms and electrons, whereas resonance structures differ *only* in the *arrangement of electrons.*

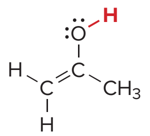
For example, ions **A** and **B** are resonance structures because the atom position is the same in both compounds, but the location of an electron pair is different. In contrast, compounds **C** and **D** are isomers because the atom placement is different; **C** has an O–H bond, and **D** has an additional C–H bond.



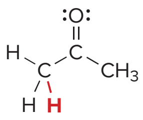
A



B



C



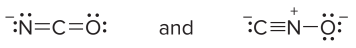
D

- **A** and **B** are **resonance** structures.
- The position of one electron pair (in red) is different.

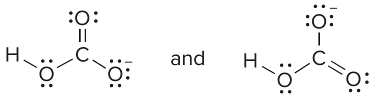
- **C** and **D** are **isomers.**
- The position of a H atom (in red) is different.

Problem 1.11 Classify each pair of compounds as isomers or resonance structures.

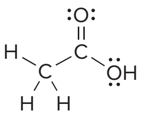
a.



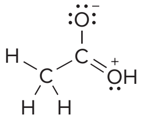
b.



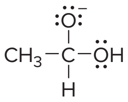
Problem 1.12 Considering structures **A–D,** classify each pair of compounds as isomers, resonance structures, or neither: (a) **A** and **B;** (b) **A** and **C;** (c) **A** and **D;** (d) **B** and **D.**



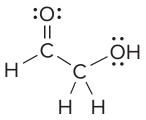
A



B



C

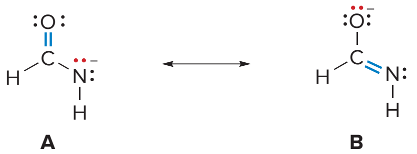


D

1.6B Drawing Resonance Structures

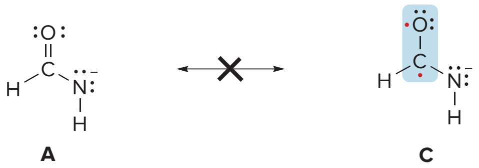
To draw resonance structures, use three criteria.

Rule [1] **Two resonance structures differ in the position of multiple bonds and nonbonded electrons. The placement of atoms and single bonds always stays the same.**



- The position of a double bond (in blue) is different.
- The position of a lone pair (in red) is different.

Rule [2] **Two resonance structures must have the same number of unpaired electrons.**

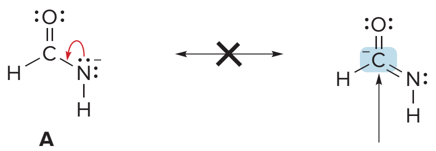


no unpaired electrons

two unpaired electrons

not a resonance structure of **A** (or **B**)

Rule [3] **Resonance structures must be valid Lewis structures. Hydrogen must have two electrons, and a second-row element can have no more than *eight* electrons.**



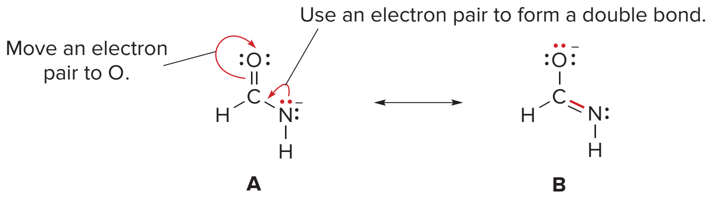
10 electrons around C

not a valid resonance structure of **A**

Curved arrow notation is a convention that shows how electron position differs between the two resonance forms.

- *Curved arrow notation shows the movement of an electron pair.* The tail of the arrow always begins at an electron pair, in either a bond or lone pair. The head points to where the electron pair "moves."

A curved arrow always begins at an electron pair. It ends at an atom or a bond.

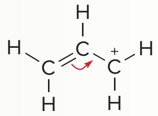

Move an electron pair to O.

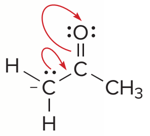
Use an electron pair to form a double bond.

Resonance structures **A** and **B** differ in the location of *two* electron pairs, so *two* curved arrows are needed. To convert **A** to **B,** take the lone pair on N and form a double bond between C and N. Then, move an electron pair in the C–O double bond to form a lone pair on O. Curved arrows thus show how to reposition the electrons in converting one resonance form to another. **The electrons themselves do not actually move.** Sample Problem 1.4 illustrates the use of curved arrows to convert one resonance structure to another.

Sample Problem 1.4 Using Curved Arrows

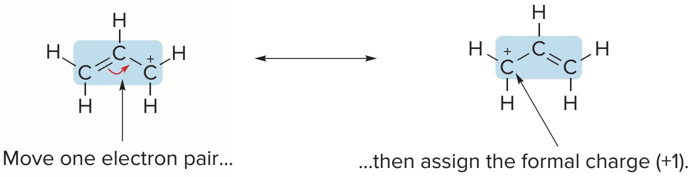
Follow the curved arrows to draw a second resonance structure for each ion.

a. 

b. 

Solution

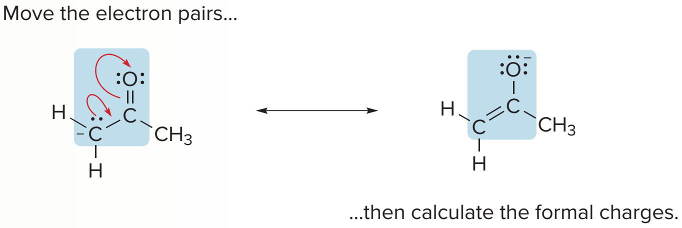
a. The curved arrow tells us to move **one** electron pair in the double bond to the adjacent C–C bond. Then determine the formal charge on any atom whose bonding is different.


Move one electron pair...

...then assign the formal charge (+1).

Positively charged carbon atoms are called **carbocations.** Carbocations are unstable intermediates because they contain a carbon atom that is lacking an octet of electrons.

b. **Two** curved arrows tell us to move **two** electron pairs. The second resonance structure has a formal charge of (–1) on O.

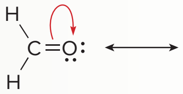

Move the electron pairs...

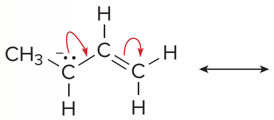
...then calculate the formal charges.

This type of resonance-stabilized anion is called an **enolate anion.** Enolates are important intermediates in many organic reactions, and all of Chapters 17 and 18 is devoted to their preparation and reactions.

Problem 1.13

Follow the curved arrows to draw a second resonance structure for each species.

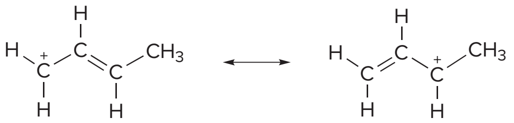
a. 

b. 

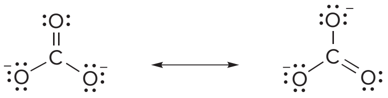
More Practice: Try Problems 1.52, 1.53.

Problem 1.14 Use curved arrow notation to show how the first resonance structure can be converted to the second.

a.

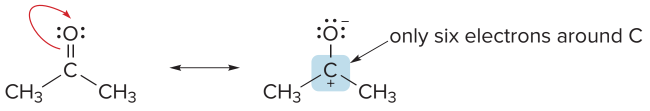


b.



Two resonance structures can have exactly the same kinds of bonds, as they do in the carbocation in Sample Problem 1.4a, or they may have different types of bonds, as they do in the enolate in Sample Problem 1.4b. Either possibility is fine as long as the individual resonance structures are valid Lewis structures.

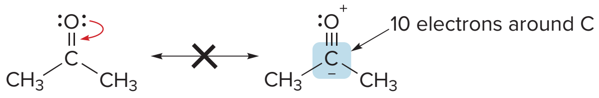
A resonance structure can have an atom with *fewer* than eight electrons around it. **B** is a resonance structure of **A** even though the carbon atom is surrounded by only six electrons.



A **B**

valid resonance structure

In contrast, a resonance structure can *never* have a second-row element with more than eight electrons. **C** is *not* a resonance structure of **A** because the carbon atom is now surrounded by 10 electrons.



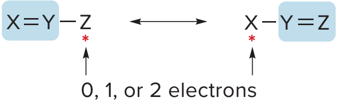
A **C**

not a valid resonance structure

We will learn much more about resonance in Chapter 12.

The ability to draw and manipulate resonance structures is a necessary skill that will be used throughout your study of organic chemistry. With practice, you will begin to recognize certain common bonding patterns for which more than one Lewis structure can be drawn. For instance, both the carbocation in Sample Problem 1.4a and the enolate anion in Sample Problem 1.4b are specific examples of one general type of resonance observed in certain three-atom systems.

- **In a group of three atoms having a multiple bond X=Y joined to an atom Z having a *p* orbital with zero, one, or two electrons, two resonance structures can be drawn.**



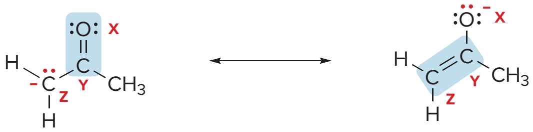
The * corresponds to a charge, a lone pair, or a single electron.

* = +, –, ·, or :

Recall from the Prologue that a ***heteroatom*** **is an atom other than carbon or hydrogen.**

X, Y, and Z may all be carbon atoms or they may be **heteroatoms** such as nitrogen and oxygen. The atom Z can be charged (positive or negative) or neutral (with a lone pair or a single electron), corresponding to the [*] in the general structure X=Y–Z*. The two resonance structures differ in the location of the multiple bond and the [*].

In the enolate anion in Sample Problem 1.4b, X corresponds to oxygen and [*] is a lone pair, which gives carbon a net negative charge. Moving the double bond and the lone pair and readjusting charges gives the second resonance structure.

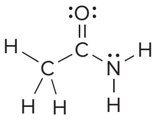


- The position of the double bond changes.
- The location of a lone pair changes.

In Chapter 12, we will learn more about the orbitals involved in this type of resonance.

Sample Problem 1.5 Drawing Resonance Structures

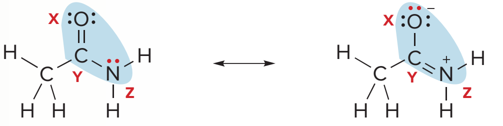
Draw a second resonance structure for acetamide.



acetamide

Solution

Always look for a three-atom system that contains a multiple bond joined to an atom Z with zero, one, or two nonbonded electrons. **Move the double bond (from X=Y to Y=Z)** and **move the [*] from Z to X.** Recalculate formal charges on X and Z.

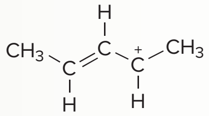


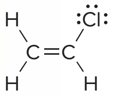
acetamide
- C=O
- lone pair on N

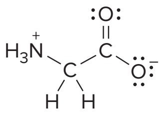
second resonance structure
- C=N
- additional lone pair on O

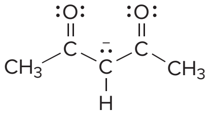
In this example, the three-atom system for resonance (X=Y–Z*) is O=C–N with a lone pair on N. After moving the double bond and the lone pair, the formal charges on O and N are –1 and +1, respectively, calculated using the procedure for determining formal charges.

Problem 1.15 Draw a second resonance structure for each species in parts (a), (b), and (c). Draw two additional resonance structures for the ion in part (d).

a.


b.


c.


d.


More Practice: Try Problems 1.54, 1.55.

1.6C The Resonance Hybrid

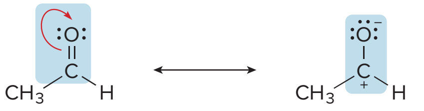
The **resonance hybrid** is the composite of all possible resonance structures. In the resonance hybrid, the electron pairs drawn in different locations in individual resonance structures are ***delocalized.***

- **The resonance hybrid is more stable than any resonance structure because it delocalizes electron density over a larger volume.**

What does the hybrid look like? When all resonance forms are identical, as they were in the carbocation in Sample Problem 1.4a, each resonance form contributes **equally** to the hybrid.

When two resonance structures are different, the hybrid looks more like the “better” resonance structure. The “better” resonance structure is called the **major contributor** to the hybrid, and all others are **minor contributors.** The hybrid is the weighted average of the contributing resonance structures. What makes one resonance structure “better” than another? There are many factors, but for now, we will learn one fact.

- A “better” resonance structure is one that has *more bonds* and *fewer charges.*



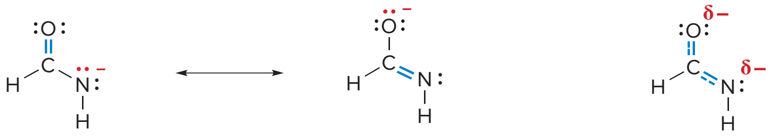
X
more bonds
fewer charges

major contributor

Y
minor contributor

Comparing resonance structures **X** and **Y, X** is the major contributor because it has more bonds and fewer charges. Thus, the hybrid looks more like **X** than **Y.**

How can we draw a hybrid, which has delocalized electron density? First, we must determine what is different in the resonance structures. Two differences commonly seen are the **position of a multiple bond** and the **site of a charge.** The anion $(HCONH)^-$ illustrates two conventions for drawing resonance hybrids.



A **B**

individual resonance structures

resonance hybrid

- The (–) charge is delocalized on N and O.
- The double bond is delocalized between O, C, and N.

Common symbols and conventions used in organic chemistry are summarized in Appendix B.

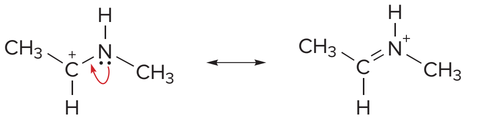
- **Double bond position. Use a dashed line for a bond that is single in one resonance structure and double in another.**
- **Location of charge. Use a δ– (partial negative charge) or δ+ (partial positive charge) for an atom that is neutral in one resonance structure and charged in another.**

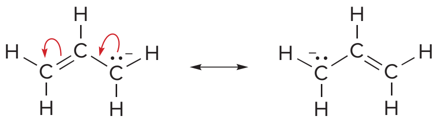
The hybrid for $(HCONH)^-$ shows two dashed bonds, indicating that both the C—O and C—N bonds have partial double bond character. Both the O and N atoms bear a partial negative charge (δ–) because these atoms are neutral in one resonance structure and negatively charged in the other.

This discussion of resonance is meant to serve as an introduction only. You will learn many more facets of resonance theory in later chapters. In Chapter 2, for example, the enormous effect of resonance on acidity is discussed.

Problem 1.16

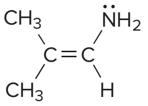
Label the resonance structures in each pair as major, minor, or equal contributors to the hybrid. Then draw the hybrid.

a.


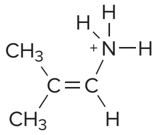
b.


Problem 1.17

(a) Draw a second resonance structure for **A.** (b) Why can't a second resonance structure be drawn for **B?**



A



B

1.7 Determining Molecular Shape

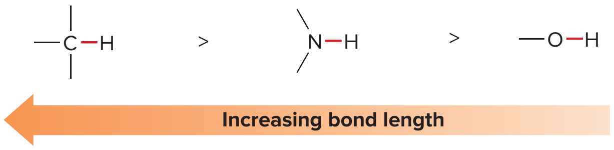
Consider the H_2O molecule. The Lewis structure tells us which atoms are connected to each other, but it implies nothing about the geometry. What does the overall molecule look like? Is H_2O a bent or linear molecule? Two variables define a molecule's structure: **bond length** and **bond angle.**

1.7A Bond Length

***Bond length* is the average distance between the centers of two bonded nuclei.** Bond lengths are typically reported in picometers (pm), where 1 pm = 10^{-12} m. For example, the O–H bond length in H_2O is 95.8 pm. Average bond lengths for common bonds are listed in Table 1.2.

Although the SI unit for bond length is the picometer (pm), the angstrom (Å) is still widely used in the chemical literature; 1 Å = 10^{-10} m. As a result, 1 pm = 10^{-2} Å, and 95.8 pm = 0.958 Å.

- Bond length *decreases* across a row of the periodic table as the size of the atom *decreases.*



- Bond length *increases* down a column of the periodic table as the size of an atom *increases.*

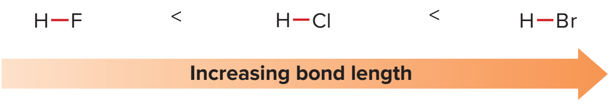


Table 1.2 Average Bond Lengths

Bond	Length (pm)	Bond	Length (pm)	Bond	Length (pm)
H–H	74	H–F	92	C–F	133
C–H	109	H–Cl	127	C–Cl	177
N–H	101	H–Br	141	C–Br	194
O–H	96	H–I	161	C–I	213

1.7B Bond Angle

Bond angle determines the shape around any atom bonded to two other atoms. To determine the bond angle and shape around a given atom, first count how many groups surround the atom. **A group is either an atom or a lone pair of electrons.** Then use the **valence shell electron pair repulsion (VSEPR) theory** to determine the shape. VSEPR is based on the fact that electron pairs repel each other; thus:

- The most stable arrangement keeps the groups around an atom as far away from each other as possible.

A second-row element has only three possible arrangements, defined by the number of groups surrounding it.

To determine geometry: [1] Draw a valid Lewis structure; [2] count groups around a given atom.

Number of groups	Geometry	Bond angle
• **two** groups	**linear**	180°
• **three** groups	**trigonal planar**	120°
• **four** groups	**tetrahedral**	109.5°

Let's examine several molecules to illustrate this phenomenon. We first need a valid Lewis structure, and then we count groups around a given atom to predict its geometry.

Two Groups Around an Atom

Any atom surrounded by only two groups is linear and has a bond angle of 180°. For example, each carbon atom in **HC≡CH** (acetylene) is surrounded by two atoms and no lone pairs, so each H—C—C bond angle in acetylene is 180°. Therefore all four atoms in HC≡CH are linear.

two atoms around each C

ball-and-stick model

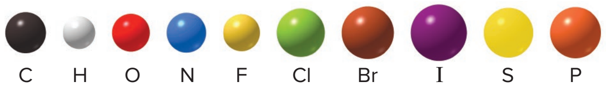
two groups
linear carbons

Most students in organic chemistry find that building models helps them visualize the shape of molecules. Invest in a set of models *now*.

Common element colors are also shown in Appendix B.

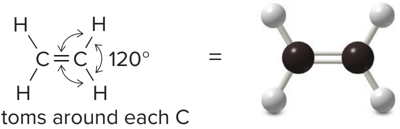
Acetylene illustrates an important feature: ***ignore multiple bonds in predicting geometry.* Count only atoms and lone pairs.**

We will represent molecules with models having balls for atoms and sticks for bonds, as in the ball-and-stick model of acetylene just shown. These representations are analogous to a set of molecular models. Balls are color-coded using accepted conventions: carbon (black), hydrogen (white or gray), oxygen (red), and so forth, as shown.



Three Groups Around an Atom

Any atom surrounded by three groups is trigonal planar and has bond angles of 120°. For example, each carbon atom in **$CH_2{=}CH_2$** (ethylene) is surrounded by three atoms and no lone pairs, making *each* H—C—C bond angle 120°. All six atoms of $CH_2{=}CH_2$ lie in one plane.



three atoms around each C

ethylene

three groups
trigonal planar carbons

Four Groups Around an Atom

Any atom surrounded by four groups is tetrahedral and has bond angles of approximately 109.5°. The simple organic compound methane, **CH_4,** has a central carbon atom with bonds to four hydrogen atoms, each pointing to a corner of a tetrahedron. This arrangement keeps four groups farther apart than a square planar arrangement in which all bond angles would be only 90°.

preferred geometry
larger H−C−H bond angle

square planar arrangement
This geometry does ***not*** occur.

four groups
tetrahedral molecule

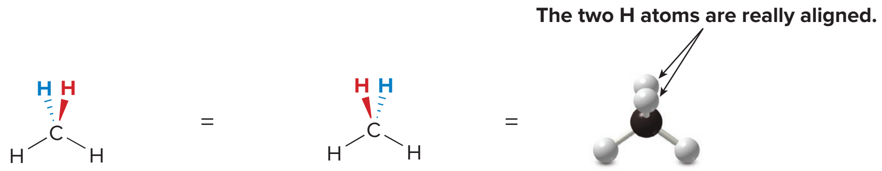
How can we represent the three-dimensional geometry of a tetrahedron on a two-dimensional piece of paper? **Place two of the bonds in the plane of the paper, one bond in front and one bond behind,** using the following conventions:

- A *solid line* is used for a bond *in* the plane.
- A *wedge* is used for a bond *in front* of the plane.
- A *dashed wedge* is used for a bond *behind* the plane.

This is just one way to draw a tetrahedron for CH_4. We can turn the molecule in many different ways, generating many equivalent representations. All of the following are acceptable drawings for CH_4, because each drawing has two solid lines, one wedge, and one dashed wedge.

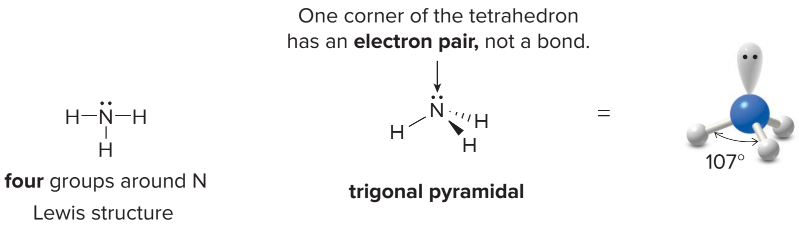
Finally, **wedges and dashed wedges are used for groups that are really *aligned one behind another.*** It does not matter in the following two drawings whether the wedge or dashed wedge is skewed to the left or right, because the two H atoms are really aligned as shown in the three-dimensional model.

All carbons in stable molecules are ***tetravalent,*** but the geometry varies with the number of groups around the particular carbon.



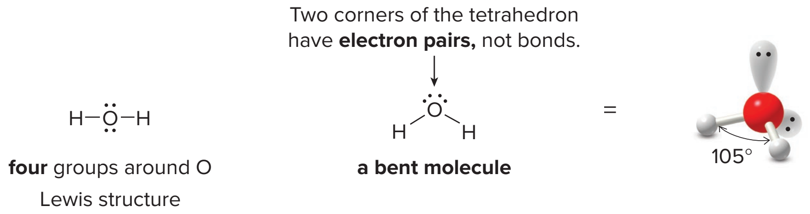
- These representations are equivalent.
- The wedge can be skewed to the left or the right of the dashed wedge.

Ammonia (NH_3) and water (H_2O) both have atoms surrounded by four groups, some of which are lone pairs. In **NH_3,** the three H atoms and one lone pair around N point to the corners of a tetrahedron. The H—N—H bond angle of 107° is close to the theoretical tetrahedral bond angle of 109.5°. This molecular shape is referred to as **trigonal pyramidal,** because one of the groups around the N is a nonbonded electron pair, not another atom.



In **H_2O,** the two H atoms and two lone pairs around O point to the corners of a tetrahedron. The H—O—H bond angle of 105° is close to the theoretical tetrahedral bond angle of 109.5°.

Water has a **bent** molecular shape, because two of the groups around oxygen are lone pairs of electrons.



In both NH_3 and H_2O, the bond angle is somewhat smaller than the theoretical tetrahedral bond angle because of repulsion of the lone pairs of electrons. The bonded atoms are compressed into a smaller space with a smaller bond angle.

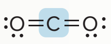
Predicting geometry based on counting groups is summarized in Table 1.3.

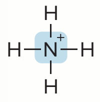
Table 1.3 Summary: Determining Geometry Based on the Number of Groups

Number of groups around an atom	Geometry	Bond angle	Examples
2	linear	180°	$HC{\equiv}CH$
3	trigonal planar	120°	$CH_2{=}CH_2$
4	tetrahedral	109.5°	CH_4, NH_3, H_2O

Sample Problem 1.6 Determining the Geometry Around a Second-Row Atom

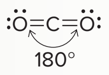
Determine the geometry around the highlighted atom in each species.

a. 

b. 

Solution

a.

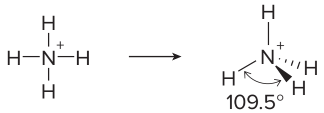


two atoms around C
no lone pairs

two groups

linear

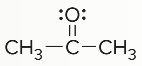
b.



four atoms around N
no lone pairs

four groups → **tetrahedral**

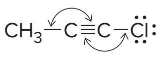
Problem 1.18 Determine the geometry around all second-row elements in each compound drawn as a Lewis structure with no implied geometry.

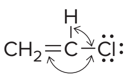
a. 

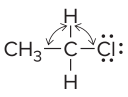
b. $CH_3{-}\ddot{\underset{\cdot\cdot}{O}}{-}CH_3$ c. $^{-}{:}\ddot{N}H_2$ d. $CH_3{-}C{\equiv}N{:}$

More Practice: Try Problems 1.60, 1.61, 1.77c, 1.79b.

Problem 1.19 Predict the indicated bond angles in each compound drawn as a Lewis structure with no implied geometry.

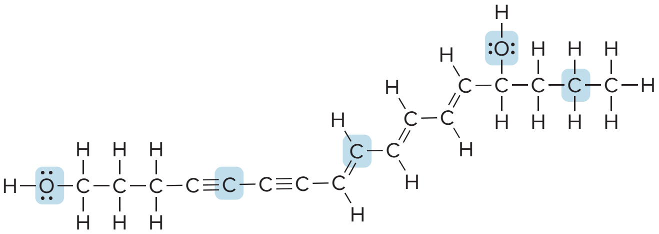
a. 

b. 

c. 

Water hemlock, which grows in wet marshy areas in the western part of North America, is the source of cicutoxin (Problem 1.20), a convulsant toxic to both livestock and humans. *Steven P. Lynch*

Problem 1.20 Using the principles of VSEPR theory, you can predict the geometry around any atom in any molecule, no matter how complex. Cicutoxin is a poisonous compound isolated from water hemlock, a highly toxic plant that grows in temperate regions in North America. Predict the geometry around the highlighted atoms in cicutoxin.



cicutoxin

1.8 Drawing Organic Structures

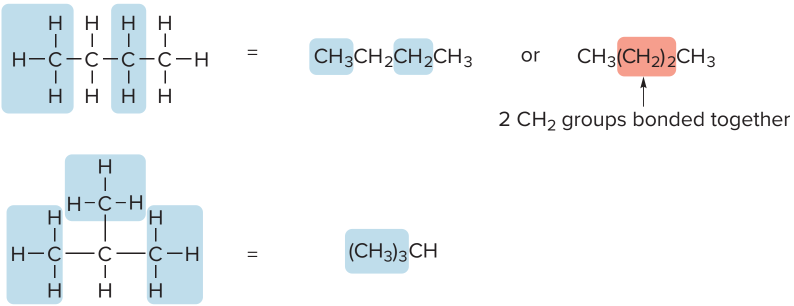
Drawing organic molecules presents a special challenge. Because they often contain many atoms, we need shorthand methods to simplify their structures. The two main types of shorthand representations used for organic compounds are **condensed structures** and **skeletal structures.**

1.8A Condensed Structures

Condensed structures can be used for compounds having a chain of atoms bonded together. The following conventions are used:

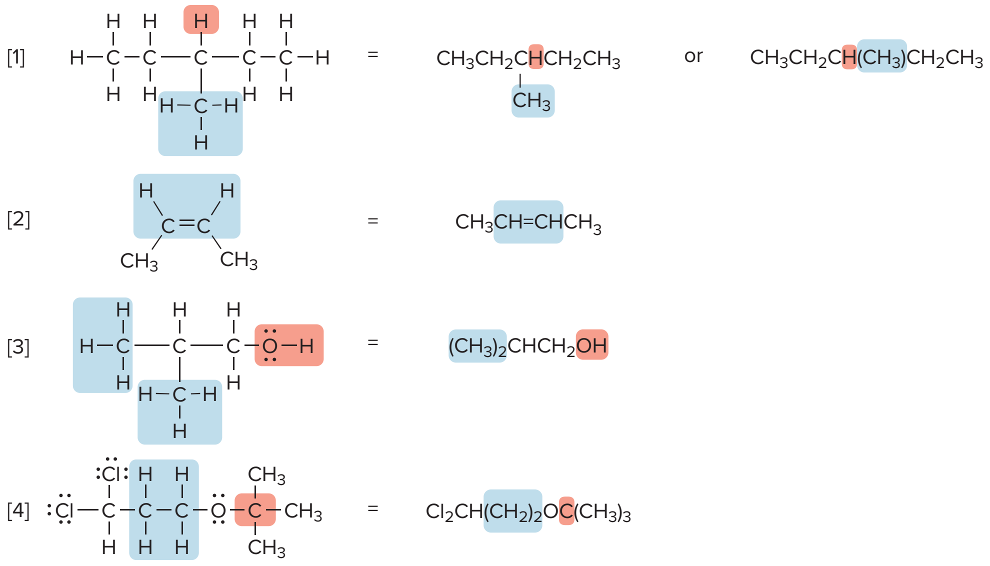
- All of the atoms are drawn in, but the two-electron bond lines are generally omitted.
- Atoms are usually drawn next to the atoms to which they are bonded.
- Parentheses are used around similar groups bonded to the same atom.
- Lone pairs are omitted.

To interpret a condensed formula, it is usually best to start at the *left side* of the molecule and remember that the ***carbon atoms must be tetravalent.*** A carbon bonded to three H atoms becomes **CH_3;** a carbon bonded to two H atoms becomes **CH_2;** and a carbon bonded to one H atom becomes **CH.**



Other examples of condensed structures with heteroatoms and carbon–carbon multiple bonds are given in Figure 1.3.

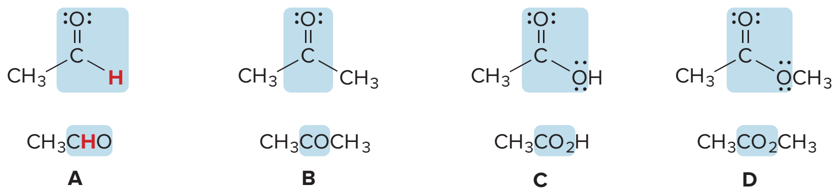
Figure 1.3 Examples of condensed structures



- Entry [1]: Draw the H atom next to the C to which it is bonded, and use parentheses around CH_3 to show it is bonded to the carbon chain.
- Entry [2]: Keep the carbon–carbon double bond and draw the H atoms after each C to which they are bonded.
- Entry [3]: Omit the lone pairs on the O atom in the condensed structure.
- Entry [4]: Omit the lone pairs on Cl and O and draw the two CH_2 groups as $(CH_2)_2$.

Translating some condensed formulas is not obvious, and it will come only with practice. This is especially true for compounds containing a carbon–oxygen double bond. Some noteworthy examples in this category are given in Figure 1.4. Whereas carbon–carbon double bonds are generally drawn in condensed structures, carbon–oxygen double bonds are usually omitted.

Figure 1.4 Condensed structures containing a C–O double bond



- In **A,** the **H** atom is bonded to C, *not* O.
- In **B,** each CH_3 group is bonded to C, *not* O.
- In **C** and **D,** the C atom is doubly bonded to one O and singly bonded to the other O.

Sample Problem 1.7 Converting a Condensed Structure to a Lewis Structure

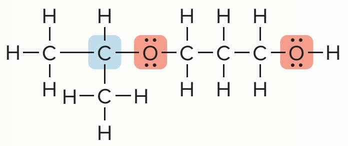
Convert each condensed formula to a Lewis structure.

a. $(CH_3)_2CHOCH_2CH_2CH_2OH$ b. $CH_3(CH_2)_2CO_2C(CH_3)_3$

Solution

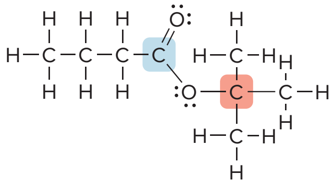
Start at the left and proceed to the right, making sure that each carbon has four bonds. Give each O atom two lone pairs to have an octet.

a. $(CH_3)_2CHOCH_2CH_2CH_2OH$



One C atom (labeled in blue) is bonded to 2 CH_3's, 1 H, and 1 O.

b. $CH_3(CH_2)_2CO_2C(CH_3)_3$



One C atom (labeled in blue) is bonded to both O's.

In part (a), the O atom is singly bonded to two C's, whereas in part (b), a C=O is needed to give each C and O an octet.

Problem 1.21 Convert each condensed formula to a Lewis structure.

a. $CH_3(CH_2)_4CH(CH_3)_2$
b. $(CH_3)_3CCH(OH)CH_2CH_3$
c. $(CH_3)_2CHCHO$
d. $(HOCH_2)_2CH(CH_2)_3C(CH_3)_2CH_2CH_3$

More Practice: Try Problems 1.64a–c, 1.65.

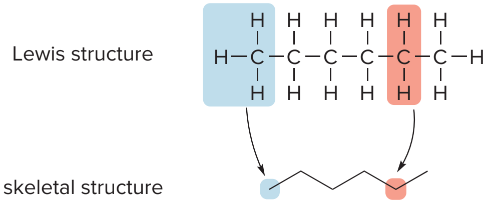
Problem 1.22 During periods of strenuous exercise, the buildup of lactic acid [$CH_3CH(OH)CO_2H$] causes the aching feeling in sore muscles. Convert this condensed structure to a Lewis structure of lactic acid.

1.8B Skeletal Structures

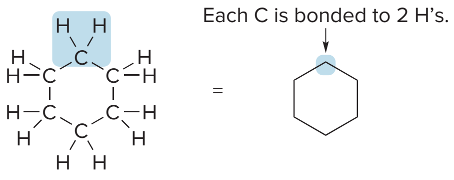
Skeletal structures are used for organic compounds containing both rings and chains of atoms. Three rules are used to draw them.

- **Assume a carbon atom is located at the junction of any two lines or at the end of any line.**
- **Assume each carbon has enough hydrogens to make it tetravalent.**
- **Draw in all heteroatoms and the hydrogens directly bonded to them.**

Carbon chains are drawn in a **zigzag** fashion, and rings are drawn as **polygons,** as shown for hexane and cyclohexane.



hexane

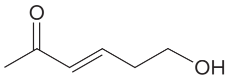


Lewis structure
C_6H_{12}

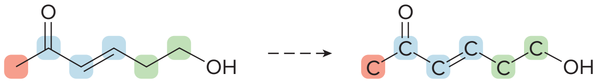
skeletal structure
cyclohexane

How To Interpret a Skeletal Structure

Example Draw in all C atoms, H atoms, and lone pairs in the following molecule:

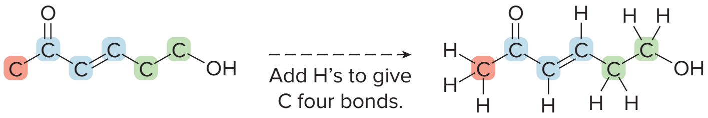


Step [1] **Place a C atom at the intersection of any two lines and at the end of any line.**



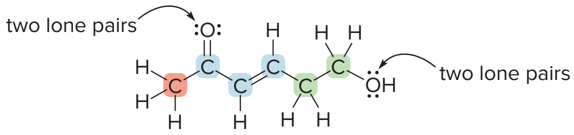
- This molecule has six carbons, including the C labeled in red at the left end of the chain.
- There are two C's (labeled in green) between the C=C and the OH group.

Step [2] **Add enough H's to make each C tetravalent.**



- The end C labeled in red needs three H's to be tetravalent.
- Each C on the C=C has three bonds already, so only one H must be drawn.
- There are two CH_2 groups between the C=C and the OH group.

Step [3] **Add lone pairs to give each heteroatom an octet.**

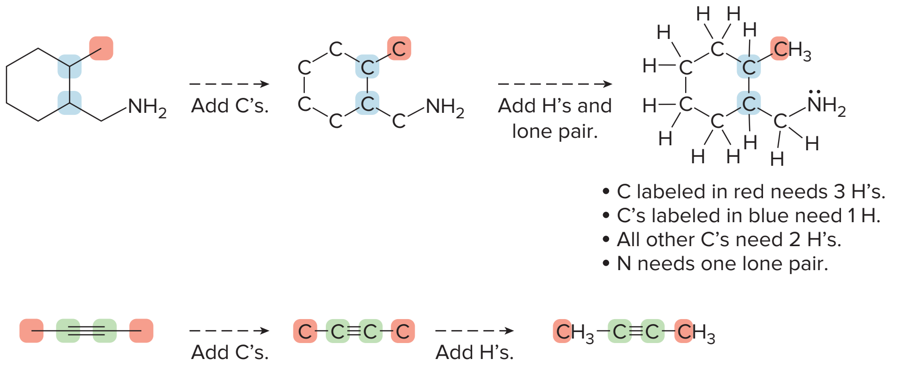


Each O needs **two** lone pairs for an octet.

Figure 1.5 shows other examples of skeletal structures, and Sample Problem 1.8 illustrates how to interpret the skeletal structure for a more complex cyclic compound.

Figure 1.5

Interpreting skeletal structures

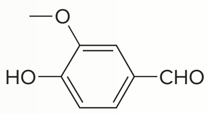


- C labeled in red needs 3 H's.
- C's labeled in blue need 1 H.
- All other C's need 2 H's.
- N needs one lone pair.

- C's labeled in red need 3 H's.
- C's labeled in green have four bonds to C.

Sample Problem 1.8 Converting a Skeletal Structure to a Lewis Structure

Draw a complete structure for vanillin showing all C atoms, H atoms, and lone pairs, and give the molecular formula. Vanillin is the principal component of the extract of the vanilla bean.



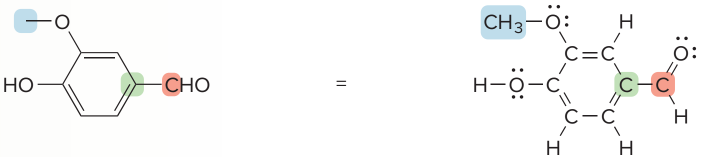
vanillin

vanilla bean

Vast natalia/Alamy Stock Photo

Solution

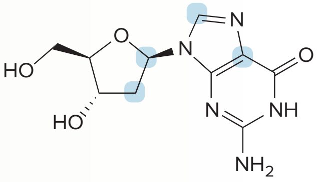
- Skeletal structures have a C atom at the junction of any two lines and at the end of any line.
- Each C must have enough H's to make it tetravalent.
- Each O atom needs two lone pairs to have a complete octet.



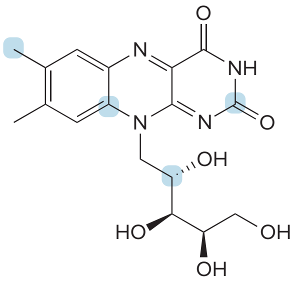
- C in blue has three H's.
- C in green has four bonds to other C's.
- C in red is doubly bonded to O.

$C_8H_8O_3$

Problem 1.23 How many hydrogen atoms are present around each highlighted carbon atom in the following molecules? What is the molecular formula for each molecule? 2'-Deoxyguanosine is a component of DNA, and riboflavin (vitamin B_2) is a yellow, water-soluble vitamin obtained in the diet from leafy greens, soybeans, almonds, and liver.

a. 

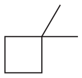
2'-deoxyguanosine
DNA component

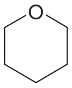
b. 

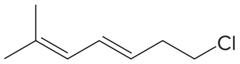
riboflavin
vitamin B_2

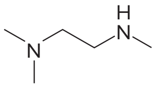
More Practice: Try Problems 1.62, 1.63, 1.80a.

Problem 1.24 Convert each skeletal structure to a complete structure with all C's, H's, and lone pairs drawn in.

a. 

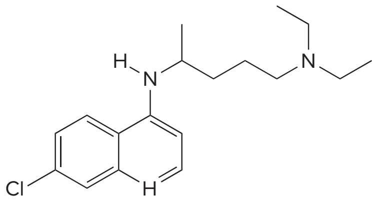
b. 

c. 

d. 

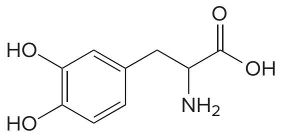
Problem 1.25 What is the molecular formula of each drug?

a.



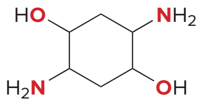
chloroquine
(antimalarial medication)

b.

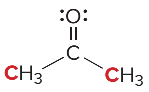


L-dopa
(drug used for Parkinson's disease)

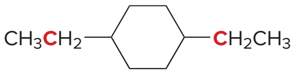
When heteroatoms are bonded to a carbon skeleton, the **heteroatom is joined *directly* to the carbon to which it is bonded,** with no H atoms in between. Thus, an OH group is drawn as OH or HO depending on where the OH is located. In contrast, when carbon appendages are bonded to a carbon skeleton, the **H atoms will be drawn to the *right* of the carbon to which they are bonded regardless of the location.**



Place the O and N atoms *directly* joined to the ring.



Two C atoms in red are bonded to the middle C.

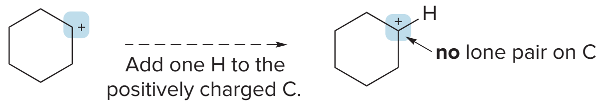


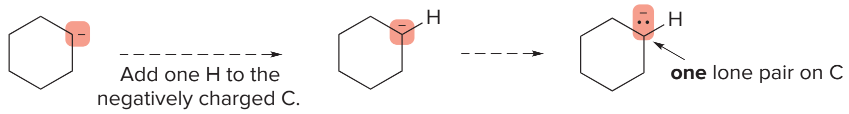
Two C atoms in red are bonded to the ring.

1.8C Skeletal Structures with Charged Atoms

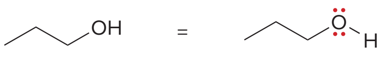
Take care in interpreting skeletal structures for positively and negatively charged carbon atoms, because *both* the hydrogen atoms *and* the lone pairs are omitted. Keep in mind the following:

- **A charge on a carbon atom takes the place of one hydrogen atom.**
- **The charge determines the number of lone pairs. Negatively charged carbon atoms have one lone pair and positively charged carbon atoms have none.**





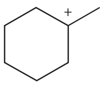
Skeletal structures often leave out lone pairs on heteroatoms, but *don't forget about them.* Use the formal charge on an atom to determine the number of lone pairs. For example, a neutral O atom with two bonds needs two additional lone pairs, and a positively charged O atom with three bonds needs only one lone pair.

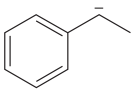


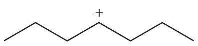
neutral O atom
two lone pairs

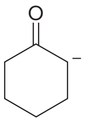
positively charged O atom
one lone pair

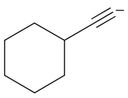
Problem 1.26 Draw in all hydrogens and lone pairs on the charged carbons in each ion.

a.


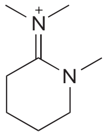
b.


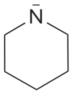
c.


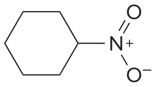
d.


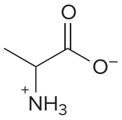
e.


Problem 1.27 Use the formal charge to draw in the lone pairs on each N or O atom in the following compounds.

a.


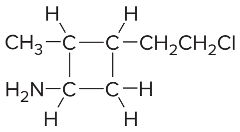
b.


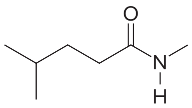
c.


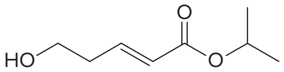
d.


Problem 1.28 Draw a skeletal structure for the molecules in parts (a) and (b), and a condensed structure for the molecules in parts (c) and (d).

a. $CH_3O(CH_2)_2COCH{=}C(CH_3)_2$

b.


c.


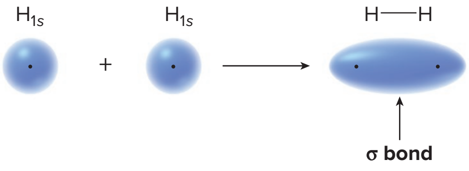
d.


1.9 Hybridization

What orbitals do the first- and second-row atoms use to form bonds?

1.9A Hydrogen

Recall from Section 1.2 that two hydrogen atoms share each of their electrons to form H_2. Thus, the 1*s* orbital on one H overlaps with the 1*s* orbital on the other H to form a bond that concentrates electron density between the two nuclei. This type of bond, called a **σ** (sigma) **bond,** is cylindrically symmetrical because the electrons forming the bond are distributed symmetrically about an imaginary line connecting the two nuclei.

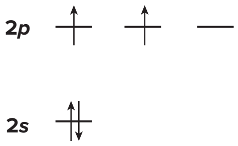


- **A σ bond concentrates electron density on the axis that joins two nuclei. All single bonds are σ bonds.**

1.9B Bonding in Methane

To account for the bonding patterns observed in more complex molecules, we must take a closer look at the 2*s* and 2*p* orbitals of atoms of the second row. Let's illustrate this with methane, CH_4.

Carbon has **four valence electrons.** To fill atomic orbitals in the most stable arrangement, electrons are placed in the orbitals of lowest energy. For carbon, this places two electrons in the 2*s* orbital and one each in two 2*p* orbitals.



ground state for
carbon's four valence electrons

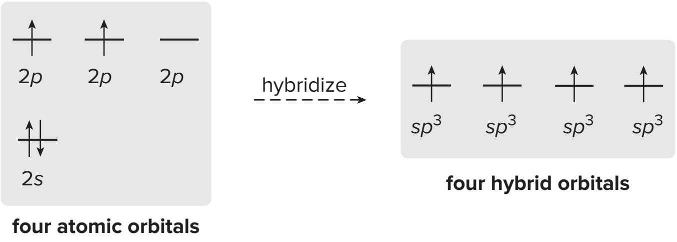
- This lowest-energy arrangement of electrons for an atom is called its **ground state.**

In this description, **carbon should form *only two* bonds** because it has only two unpaired valence electrons, and CH_2 should be a stable molecule. In reality, however, CH_2 is a highly reactive species because carbon does not have an octet of electrons.

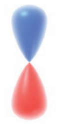
Because the carbon atom in CH_4 forms four bonds to hydrogen and **all C—H bonds are *identical,*** chemists have proposed that atoms like carbon do *not* use pure *s* and pure *p* orbitals in forming bonds. Instead, atoms use a set of new orbitals called **hybrid orbitals.** The mathematical process by which these orbitals are formed is called **hybridization.**

- ***Hybridization* is the combination of two or more atomic orbitals to form the same number of hybrid orbitals, each having the same shape and energy.**

Hybridization of *one* 2*s* orbital and *three* 2*p* orbitals for carbon forms *four* hybrid orbitals, each with one electron. These new hybrid orbitals are intermediate in energy between the 2*s* and 2*p* orbitals.

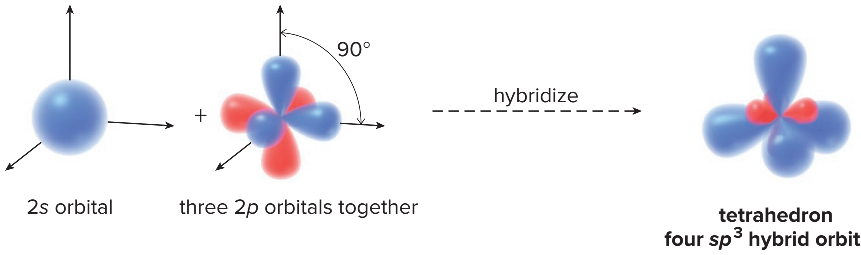


- **These hybrid orbitals are called *sp*^{3} *hybrids* because they are formed from *one s* orbital and *three p* orbitals.**


p orbital


***sp*^{3}** hybrid orbital

What do these new hybrid orbitals look like? Mixing a spherical 2*s* orbital and three dumbbell-shaped 2*p* orbitals together produces four orbitals having one large lobe and one small lobe, oriented toward the corners of a tetrahedron. Each large lobe concentrates electron density in the bonding direction between two nuclei. **Bonds formed from hybrid orbitals are *stronger* than bonds formed from pure *p* orbitals.**

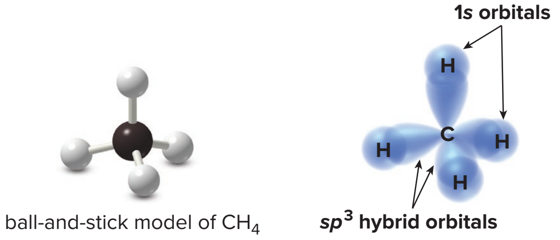


The four hybrid orbitals form four equivalent bonds. We can now explain the observed bonding in CH_4.

- **Each bond in CH_4 is formed by overlap of an *sp*^{3} hybrid orbital of carbon with a 1*s* orbital of hydrogen. These four bonds point to the corners of a tetrahedron.**

All four C—H bonds in methane are **σ bonds,** because the electron density is concentrated on the axis joining C and H. An orbital picture of the bonding in CH_4 is given in Figure 1.6.

Figure 1.6
Bonding in CH_4 using *sp*^{3} hybrid orbitals



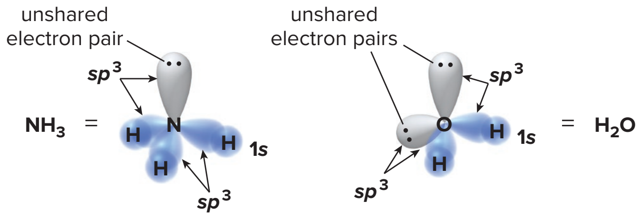
- All four C—H bonds are σ bonds. Each is formed by overlap of an *sp*^{3} hybrid orbital on carbon and a 1*s* orbital on hydrogen.

Problem 1.29 What orbitals are used to form each of the C—C and C—H bonds in $CH_3CH_2CH_3$ (propane)? How many σ bonds are present in this molecule?

- **Any atom surrounded by four groups (atoms and lone pairs) is *sp*^{3} hybridized.**

The N atom in **NH_3** and the O atom in **H_2O** are both surrounded by four groups, making them *sp*^{3} hybridized. Each N—H and O—H bond in these molecules is formed by overlap of an *sp*^{3} hybrid orbital with a 1*s* orbital from H. The lone pairs of electrons on N and O also occupy *sp*^{3} hybrid orbitals, as shown in Figure 1.7.

Figure 1.7
Hybrid orbitals of NH_3 and H_2O



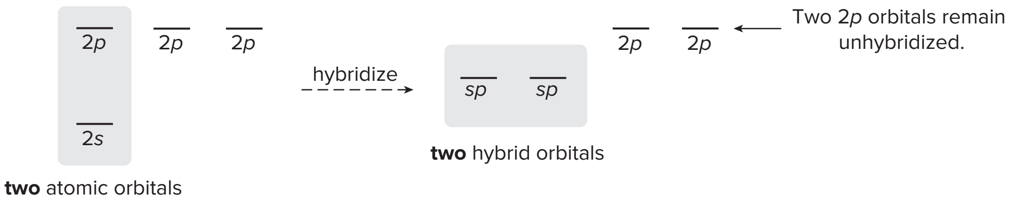
1.9C Other Hybridization Patterns—*sp* and *sp*^{2} Hybrid Orbitals

Forming *sp*^{3} hybrid orbitals is just one way that 2*s* and 2*p* orbitals can hybridize. Three common modes of hybridization are seen in organic molecules. The number of orbitals is always conserved in hybridization; that is, a **given number of atomic orbitals hybridizes to form an *equivalent* number of hybrid orbitals.**

- ***One* 2*s* orbital and *three* 2*p* orbitals form *four sp*^{3} hybrid orbitals.**
- ***One* 2*s* orbital and *two* 2*p* orbitals form *three sp*^{2} hybrid orbitals.**
- ***One* 2*s* orbital and *one* 2*p* orbital form *two sp* hybrid orbitals.**

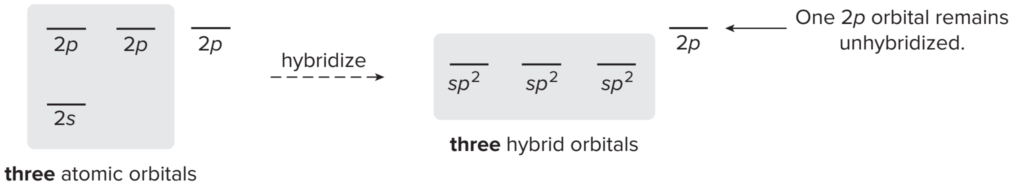
We have already seen pictorially how four *sp*^{3} hybrid orbitals are formed from one 2*s* and three 2*p* orbitals. Figures 1.8 and 1.9 illustrate the same process for *sp* and *sp*^{2} hybrids. Each *sp* and *sp*^{2} hybrid orbital has one large and one small lobe, much like an *sp*^{3} hybrid orbital. Note, however, that both *sp*^{2} and *sp* hybridization **leave one and two 2*p* orbitals *unhybridized,*** respectively, on each atom.

Figure 1.8
Forming two *sp* hybrid orbitals



- Forming **two *sp* hybrid orbitals** uses **one 2*s*** and **one 2*p* orbital,** leaving **two 2*p* orbitals *unhybridized.***

Figure 1.9
Forming three *sp*^{2} hybrid orbitals



- Forming **three *sp*^{2} hybrid orbitals** uses **one 2*s*** and **two 2*p* orbitals,** leaving **one 2*p* orbital *unhybridized.***

The **superscripts** for hybrid orbitals correspond to the **number of atomic orbitals** used to form them. The number “1” is understood.

For example: $sp^3 = s^1p^3$

one 2*s* + **three** 2*p* orbitals used to make each hybrid orbital

To determine the hybridization of an atom in a molecule, we count groups (atoms and lone pairs) around the atom, just as we did in determining geometry.

- **The number of groups around an atom *equals* the number of atomic orbitals that are hybridized to form hybrid orbitals (Table 1.4).**

Table 1.4 Three Types of Hybrid Orbitals

Number of groups	Number of orbitals used	Type of hybrid orbital
2	2	**two** *sp* hybrid orbitals
3	3	**three** sp^2 hybrid orbitals
4	4	**four** sp^3 hybrid orbitals

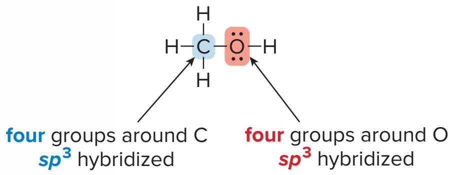
Hybridization in various carbon compounds is presented in Section 1.10.

Sample Problem 1.9 Determining the Hybridization of an Atom

What orbitals are used to form each bond in methanol, CH_3OH?

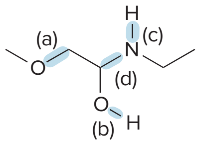
Solution

To solve this problem, **draw a valid Lewis structure** and **count groups around each atom.** Then, use the rule to determine hybridization: **two groups = *sp*, three groups = sp^2, and four groups = sp^3.**



- All C–H bonds are formed from C_{sp^3}–H_{1s}.
- The C–O bond is formed from C_{sp^3}–O_{sp^3}.
- The O–H bond is formed from O_{sp^3}–H_{1s}.

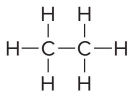
Problem 1.30 What orbitals are used to form each highlighted bond in the following molecule? In what type of orbital do the lone pairs on each O and N reside?



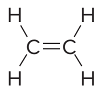
More Practice: Try Problems 1.67a–c, 1.68.

1.10 Ethane, Ethylene, and Acetylene

The principles of hybridization determine the type of bonds in **ethane, ethylene,** and **acetylene.**



ethane



ethylene

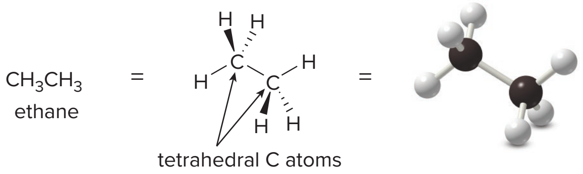
$H-C\equiv C-H$

acetylene

1.10A Ethane—CH_3CH_3

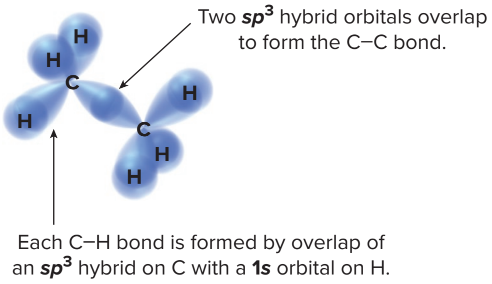
According to the Lewis structure for **ethane, CH_3CH_3,** each carbon atom is singly bonded to four other atoms. As a result:

- **Each carbon is tetrahedral.**
- **Each carbon is *sp*^{3} hybridized.**

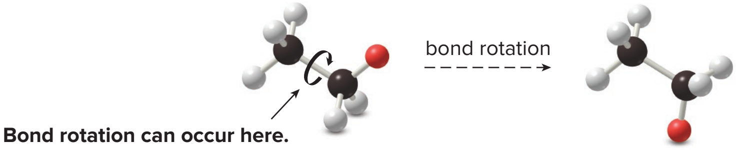


All of the bonds in ethane are σ bonds. The C—H bonds are formed from the overlap of one of the three sp^3 hybrid orbitals on each carbon atom with the 1*s* orbital on hydrogen. The C—C bond is formed from the overlap of an sp^3 hybrid orbital on each carbon atom.

Ethane is a constituent of natural gas. *Steve Allen/Brand X Pictures*



A model of ethane shows that **rotation can occur around the central C—C σ bond.** The relative position of the H atoms on the adjacent CH_3 groups changes with bond rotation, as seen in the location of the labeled red H atom before and after rotation. This process is discussed in greater detail in Chapter 4.

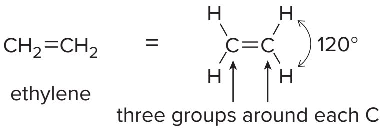


1.10B Ethylene—C_2H_4

Based on the Lewis structure of **ethylene, $CH_2{=}CH_2$,** each carbon atom is singly bonded to two H atoms and doubly bonded to the other C atom, so each C is surrounded by three groups. As a result:

Ethylene is an important starting material in the preparation of the plastic polyethylene. *Nextdoor Images/Creatas/PunchStock*

- **Each carbon is trigonal planar (Section 1.7B).**
- **Each carbon is *sp*^{2} hybridized.**



What orbitals are used to form the two bonds of the C—C double bond? Recall from Section 1.9 that ***sp*^{2} hybrid orbitals** are formed from **one 2*s* and two 2*p* orbitals,** leaving one **2*p* orbital unhybridized.** Because carbon has four valence electrons, **each of these orbitals has one electron** that can be used to form a bond.

Each C—H bond results from the end-on overlap of an sp^2 hybrid orbital on carbon and the 1*s* orbital on hydrogen. Similarly, one of the C—C bonds results from the end-on overlap of