

CHAPTER 1 | Atomic and Molecular Structure

This first chapter introduces organic chemistry and begins an organic-centered review of relevant information from general chemistry. Chapter 1 reviews atomic structure, electron configurations, covalent and ionic bonds, electronegativity, bond dipoles, bond energy, bond length, formal charge, and oxidation numbers. The chapter summarizes the stepwise approach to drawing Lewis dot structures and then introduces a method for quickly generating Lewis dot structures for organic molecules. The chapter also includes a lengthy discussion of resonance structures, including visual clues that allow students to identify when resonance structures will exist for a species and an introduction to curved arrow notation. The chapter concludes with new topics for students, including the various representations of molecules (Lewis dot structures, condensed formulas, and line drawings) and a survey of functional groups.

HEADS UP!

The temptation is always to shortchange the “review” chapters because so much new information is waiting for students in later chapters. No matter how strong your students are from their general chemistry experience, some parts should not be skipped. In several places, Karty is setting up the rest of the semester by combining concepts or presenting them in particular ways, or going deeper than you might expect for an early chapter. For example, Section 1.9 presents formal charges from a molecular approach (which differs from the mathematical formula-based approach often used in general chemistry). In addition, Karty uses energy diagrams during his discussion of resonance theory (Section 1.10) and uses energy to justify stability (and then have students predict stability) in ways that most general chemistry courses do not. He leads from there directly into electron-pushing arrows (Section 1.11) and integrates them with his discussion on formal charges. The use of both energy diagrams (qualitative or quantitative) and curved arrow notation is vital to this text.

COMMENTS BY SECTION

1.1. What Is Organic Chemistry?

1.2. Why Carbon?

1.3. Atomic Structure and Ground State Electron Configurations

The first three sections of the chapter define organic chemistry, describe carbon’s unique properties, and review atomic theory, including wave functions and electron configurations. Even here, in the first few sections, the text is using complex structures (Figure 1-2, royal purple, for example) and branching systems to help students immediately become comfortable with larger molecules.

1.4. The Covalent Bond: Bond Energy and Bond Length

Section 1.4 discusses covalent bonds. It gives students an overview of bond length, strength, and energy and the types of bonds that occur in organic chemistry. The table of bond energies (Table 1-2) is worth noting because the text will use those values in discussing bond energy as a driving force (e.g., Section 7.8). The textbook generally provides bond energy values in the discussion; however, you may wish to send students to Table 1-2 to confirm the values or to use them in assignments.

1.5. Lewis Dot Structures and the Octet Rule

Section 1.5 summarizes the typical five-step process for drawing Lewis dot structures that students learn in general chemistry. A quick review of that process is a useful way to move students into the next section.

1.6. Strategies for Success: Drawing Lewis Dot Structures Quickly

This section is the first place where students often need to start working hard because they are applying what they have learned to new situations. Students are tempted to try to memorize the information presented in Table 1-4, which summarizes the numbers of bonds and lone pairs for H, C, N, O, X (where X = F, Cl, Br, or I), and Ne atoms

with no formal charge. I always advise my students to use that table as a tool to augment the five-step process (Section 1.5) and tell them that although they should not memorize the table, they will end up knowing it by heart through simple practice.

This section, and Table 1-4 in particular, helps students make the transition from the general chemistry approach of counting valence electrons and creating a structure to the faster method of creating a structure based on the number of bond and lone pairs expected for each first-row atom. That transition is not always presented explicitly in organic chemistry textbooks, and students find it useful.

1.7. Electronegativity, Polar Covalent Bonds, and Bond Dipoles

Section 1.7 introduces polar covalent bonds and electrostatic potential diagrams; however, net dipoles are not discussed until Section 2.4. Some instructors may expect those two topics to be treated together, but this chapter is focused on individual bonds (not geometry). This chapter has enough to cover without introducing geometry, and it allows a greater focus on bonds, formal charges, and electron movement. Net dipoles are deferred until the discussion of intermolecular forces in Chapter 2.

1.8. Ionic Bonds

Section 1.8 defines ionic bonds, provides guidelines for identifying ionic compounds, and describes polyatomic anions and cations, noting that most polyatomic cations contain a nitrogen atom.

1.9. Assigning Electrons to Atoms in Molecules: Formal Charge

Section 1.9 provides a simple method to calculate formal charges and does so without presenting it in a symbolic mathematical formula. The calculation is still there, and students work it out in Your Turn 1.8, but it is calculated as the valence electrons of the atom in the molecule (lone pairs and half-bonding pairs) versus the protons of that atom. In my experience, students are used to some variation of a mathematical presentation, such as “formal charge = valence electrons in the uncharged atom – (lone pairs of the atom in the molecule + $\frac{1}{2} \times$ bonding pairs).” Students may initially be concerned that they are not “using the formula,” but they quickly adapt to the commonsense approach of looking at valence electrons of the atom *in the molecular setting* versus the protons of that atom.

1.10. Resonance Theory

Section 1.10 provides six observations about resonance contributors, with examples, that students need to know. Those observations introduce students to how we interpret resonance contributors. The section does not compare structures with negative charges on atoms of different electronegativities; that topic appears in Sections 6.7 and 6.8. Although this section introduces the concept of equivalent/inequivalent resonance contributors (major/minor contributors), the idea is developed more fully later.

1.11. Strategies for Success: Drawing All Resonance Structures

Section 1.11 summarizes the situations in which resonance contributors are possible: lone pairs adjacent to π bonds, positive charges (or lacking an octet) adjacent to π bonds or lone pairs, and aromatic structures. Those are important visual clues that students can use to determine whether resonance contributors are possible for a chemical species.

The second aspect of this section is the introduction of curved arrow notation for drawing electron flow. To start using curved arrow notation at this point is extremely worthwhile. It is a natural way to indicate electron movement, it makes resonance forms easier for students to understand, and every bit of practice put into curved arrows now will pay off handsomely in later chapters.

1.12. Shorthand Notations

Section 1.12 compares condensed formulas, Lewis structures, and line drawings. That discussion explains to students how to translate one representation into another. Table 1-5 summarizes the types of formal charges students will see. Each results from the change of a lone pair to a shared pair (or vice versa) except the formation of

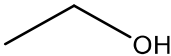
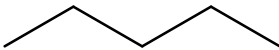
carbocations. That information, which expands on the information in Table 1-4 in Section 1.6, allows students to assess structures and provide the appropriate charges or lone pairs without calculating formal charge.

You may want to include examples with heteroatoms on the left end of the molecule and show that Hs attached to those generally do not follow the atom. Examples:

Ethylene glycol HOCH₂CH₂OH is preferable to OHCH₂CH₂OH.

Glycine H₂NCH₂COOH is preferable to NH₂CH₂COOH.

If you use discovery learning in class, you can give students a table similar to the one below and have them fill in the empty cells, using the first line of entries as a guide. In general, the line structures are the most challenging.

Molecular Formula	Structural Formula	Condensed Formula	Line Drawing
C ₂ H ₆ O	$ \begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{H}-\text{C}-\text{C}-\text{OH} \\ \quad \\ \text{H} \quad \text{H} \end{array} $	CH ₃ CH ₂ OH	
	$ \begin{array}{c} \text{H} \quad \quad \text{H} \\ \quad \quad \\ \text{H}-\text{C}-\text{O}-\text{C}-\text{H} \\ \quad \quad \\ \text{H} \quad \quad \text{H} \end{array} $		
			
		CH ₃ CH ₂ CH ₂ CH ₂ NH ₂	

1.13. An Overview of Organic Compounds: Functional Groups

Section 1.13 introduces 17 functional groups (Table 1-6), as well as some comments about differentiating functional groups. You may wish to assess the list and modify it. The list is, as described, an overview and is not comprehensive. For example, sulfides and reactive carboxylic acid derivatives are absent. Even so, it is a useful table to start with, and I have found it worthwhile to hand out the table in class as a starting point of groups that students should be able to identify by the first exam.

Identifying functional groups can be a stumbling block for students, who often interpret some complex functional groups as combinations of multiple simple ones. An ester, for example, can appear to be a ketone and an ether. In a similar vein, acetals and hemiacetals are often the hardest groups for students to identify because of their similarities to ethers and alcohols. An aryl ring can appear to be three alkene groups. Using real-world molecules, and identifying groups with the help of some table (this one or one you produce), is good practice for this chapter.

The text helpfully does not include *alkane* as a functional group. Rather, the term indicates a molecule with no functional groups present.

1.14. An Introduction to Proteins, Carbohydrates, and Nucleic Acids: Fundamental Building Blocks and Functional Groups

Sections with the heading “The Organic Chemistry of Biomolecules” appear throughout the book, and Section 1.14

is the first of those. The sections serve several purposes.

For instructors, placing that information at the ends of chapters throughout the textbook gives them the option of covering the information they wish to include. Informal surveys of instructors indicate that, historically, most organic chemistry instructors minimize the coverage of biomolecules in their courses. (Doing so is understandable because that information usually appears in chapters at the end of the textbook.)

For students, the sections offer access to information they may need. For example, in its materials documenting the changes in the Medical College Admissions Test in 2015, the Association of American Medical Colleges detailed an expectation that students learn certain aspects of biochemistry in their organic chemistry courses. Other standardized exams, such as those of the American Chemical Society, have similar expectations.

For both students and instructors, these sections present an opportunity to apply the concepts presented in the chapter in the context of biomolecules. In Chapter 1, for example, students practice identifying functional groups (presented in Section 1.13) in proteins, carbohydrates, and nucleic acids.

STUDENTS' PERSPECTIVES

The text emphasizes how important it is for students to start using curved arrow notation and line structures starting with this chapter. Having two new concepts appear in the first chapter has helped my students build good study habits during the first week of classes. These new concepts often convince students to start studying right away! Pushing these new concepts so that they start using curved arrow notation as part of their determination of resonance structures (rather than something they draw in later as an afterthought) has overwhelmingly helped student outcomes in my course. If they start “thinking arrows now,” using arrows to help them figure out what is happening, they do better in the course overall.

Apart from their first exposure to arrows, students in my course have been most challenged by taking a neutral structure and providing resonance structures that result in charges on the molecule. It is difficult for them to take something that looks complete and “happy” and convert it to a form that appears incorrect to them (with formal charges on two atoms). This sometimes leads students to struggle with distinguishing simply-foreign-looking-but-correct structures from ones that are actually incorrect. Typical mistakes involve carbon with 5 or more bonds or oxygen with 10 electrons. We need to work through a number of examples of neutral molecules before all my students are able to trust their judgements.

RESOURCES

Pharmaceuticals are a rich source of molecules for questions that require students to identify functional groups. Although you can create your own molecules, students—particularly prepharmacy and premed students—will probably be more interested in pharmaceuticals. You can browse *The Merck Index* or *Chemical and Engineering News* for examples. The structures are generally available quickly on the Internet through an image search. In the past, students have brought me large collections of the informational sheets that accompany pharmaceuticals, and I have created exam questions from those sheets.

You can also find examples at the American Chemical Society’s “Molecule of the Week” archive by going to <http://www.acs.org> and clicking “What molecule am I?” under “Molecule of the Week.”

Sometimes I find myself looking for molecules with specific functional groups for students to practice. The examples below represent a few interesting molecules and a list of the functional groups that they contain.

Molecule	Functional Groups
Atorvastatin (Lipitor)	Amide, amine, fluorine, hydroxy groups, aromatic rings, carboxylic acid
Lovastatin (Mevacor)	Esters, hydroxy group, alkenes
Zingerone (vanillylacetone)	Ketone, hydroxy group (phenol), ether, aromatic ring
Albuterol	Hydroxy groups (including phenol), amine, aromatic ring
Aspartame (NutraSweet)	Carboxylic acid, amine, amide, ester, aromatic ring
α -Damascone	Ketones, alkenes
Vanillin	Hydroxy group (phenol), ether, aldehyde, aromatic ring

Suggested Clicker Questions

The following clicker questions have been selected from the Chapter 1 Clicker Question PowerPoints available on wwnorton.com/instructors. More questions for each chapter are available at the website.

1.6. *Strategies for Success: Drawing Lewis Dot Structures Quickly*

“The connectivity of a particular molecule is shown below. Assuming that no atoms have a formal charge, how many double bonds are there in its completed Lewis structure?”

That problem asks students to apply Lewis dot rules quickly to a large (and imposing) molecule. The task is not that difficult once they consider that carbon needs to have four bonds, and it lets them see how approachable a difficult-looking problem can be with a few simple steps.

1.9. *Assigning Electrons to Atoms in Molecules: Formal Charge*

“What is the formal charge on the oxygen in the following compound?”

That problem forces students to “think outside the box” for a little bit because the formal charge on the oxygen is +1. That was often considered unusual in structures from general chemistry, but the situation is not unusual in organic chemistry.

1.10. *Resonance Theory*

“Which is not an acceptable resonance form of the boxed compound? (Choose 1–4)” and “Why is this form not acceptable? (Choose 5–8).”

That problem not only asks which resonance form is wrong but also delves deeper into why it is incorrect. The question and the follow-up question can be useful to students because sometimes they simply feel that a structure “looks wrong,” but they have no idea why.

INTERCHAPTER A | Nomenclature: The Basic System for Naming Simple Organic Compounds: Alkanes, Haloalkanes, Nitroalkanes, Cycloalkanes, and Ethers

The textbook covers nomenclature in separate interchapter sections rather than within the chapters. This section is placed right after Chapter 1 and introduces the IUPAC system as well as simple functional groups on alkanes. Students need to learn that material during the first part of the first semester because they will encounter alkanes and cycloalkanes in Chapter 4 in the context of conformation isomerism. Students will encounter haloalkanes (alkyl halides) as reactants in nucleophilic substitution and elimination reactions in Chapter 8.

HEADS UP!

Why does the text cover nomenclature in separate sections? Joel Karty explained that organization in his blog post “On Nomenclature” (posted October 16, 2012, at teachthemechanism.com). One reason is that it helps students focus as they learn. A second benefit is that separating nomenclature from the main chapters better enables students to see how the various nomenclature rules are related. Yet a third benefit comes when students review for an exam, especially a cumulative final exam. Doing so is much easier and more straightforward when the nomenclature rules are all collected together and organized logically.

COMMENTS BY SECTION

A.1. The Need for Systematic Nomenclature: An Introduction to the IUPAC System

This section sets up the reasoning behind the IUPAC system, which empowers students by letting them know that they can take an IUPAC name and use it to work out a compound’s structure once they know a few basic rules.

A.2. Alkanes and Substituted Alkanes

This section introduces the root words for alkanes (taking it to 10 carbons, Table A-1) and the concept of substituents.

A.3. Haloalkanes and Nitroalkanes: Roots, Prefixes, and Locator Numbers

This section introduces simple substituents (halogen and nitro groups) and then introduces naming substituted alkanes. Starting by using locator numbers and prefixes with halogens or nitroalkanes has been easier for me than starting with alkyl groups because alkyl groups add the complexity of locating the longest carbon chain.

A.4. Alkyl Substituents: Branched Alkanes and Substituted Branched Alkanes

This section brings alkyl substituents into play, from simple straight-chain substituents to substituted branched substituents. This section deals with all substituted branched systems by using IUPAC nomenclature, not common names (such as isopropyl), which Section A.7 deals with. If you intend students to use only common names in their branching, I advise dealing with that in class or in a handout.

A.5. Cyclic Alkanes and Cyclic Alkyl Groups

This section deals with cyclic alkanes, from three to eight carbons, as well as the rules surrounding when the cyclic is the root versus the substituent. Substituted rings, including ones with halogens or nitro groups, also are discussed. Now is a good time to introduce the idea that five-, six-, and seven-membered rings are favorable configurations for carbon.

A.6. Ethers and Alkoxy Groups

This section introduces –OR groups and the different ways that they can be named. Although including those groups now might seem unusual, this topic offers another example of substituents that do not change the suffix of the name.

A.7. Trivial Names or Common Names

The information on IUPAC nomenclature is fairly straightforward, and instructors will want students to learn most of the information. However, instructors will differ on which trivial (or common) names they wish students to learn. The list of names is extensive, and you may want to tell students that they can skip certain trivial names. You may also want to add some.

For example, I want students to use the common names for different propyl and butyl groups, especially because the *t*-butyl will be so useful synthetically, but I do not ask them to learn the names of the pentyl groups. If you choose to edit, giving students a small handout of common names that they are responsible for can be useful.

STUDENTS' PERSPECTIVES

Many instructors approach these interchapters as something that students should work through on their own. Overall, I have been surprised at how easily students master the material with minimal input from the instructor. I also recall occasions when students, having read and practiced the application of the relatively recent changes in IUPAC rules, knew more than I did about certain rules. I do recommend that you allow students the opportunity to ask questions about nomenclature during the course, and find a way (through quizzes or tests) to hold them accountable for the material to keep them honest in their independent work.

How you assess students' knowledge is up to you: a quiz for each nomenclature section, a page on an exam each semester, or the like. My colleague, for example, incorporates nomenclature into exam questions. Instead of giving students the structure of a starting material for a reaction, he supplies the IUPAC name.

If you have a small class, consider the following exercise: I give students a deliberately challenging quiz on a series of molecules, each of which the students have to name. While they complete the quiz, I put the molecules on the board. After the students turn in the quiz, I have them go to the board and name a single molecule. Then, working in groups, the students evaluate the names and recommend changes that will correct errors. I provide no input, but I do tell them what the score on the quiz would be according to what is on the board. We continue until the class comes up with names that earn a perfect score. Students have responded favorably to that approach, especially when I warn them that this level of difficulty is fair game for the exam but then surprise them with full credit to the class on that quiz after their hard work!

RESOURCES

William B. Jensen of the University of Cincinnati has written many short, historical pieces that deal with organic nomenclature and symbolism. Here is a selection of his articles:

- “The Origins of the Qualifiers Iso-, Neo-, Primary, Secondary, and Tertiary in Organic Nomenclature.” *J. Chem. Educ.* **2012**, *89*, 953–954. doi:10.1021/ed101192y.
- “Why Is ‘R’ Used to Symbolize Hydrocarbon Substituents?” *J. Chem. Educ.* **2010**, *87*, 360–361. doi:10.1021/ed800139p.
- “The Origins of the Ortho-, Meta-, and Para- Prefixes in Chemical Nomenclature.” *J. Chem. Educ.* **2006**, *83*, 356. doi:10.1021/ed083p356.
- “The Origin of Vinyl.” *J. Chem. Educ.* **2004**, *81*, 464. doi:10.1021/ed081p464.

Most textbooks don't address the pronunciation of names of organic compounds. Most spellings are created from words used in spoken language. The names of organic compounds are exceptions because these names are created first as written words through sets of rules. Consequently, instead of a spoken word's being represented by letters, a spoken word is generated from letters. That approach leads to ambiguities and variations. Some examples include the following:

- The multiple pronunciations of the functional group *amide*.
- The British pronunciations of *methyl* and other terms. For examples, view the videos by the University of Surrey on nucleophilic substitution, available on YouTube.
- The debate over the pronunciation of the *c* in *decyl*, documented by K. M. Reese in *Chem. Eng. News* **1987**, *65*, 64. doi:10.1021/cen-v065n022.p064.

You may wish to use one or more of those examples to show students that some variation is acceptable in pronouncing the names of organic compounds.

Suggested Clicker Questions

The following clicker questions have been selected from the Interchapter A Clicker Question PowerPoints available on www.norton.com/instructors. More questions for each chapter are available at the website.

A.4. Alkyl Substituents: Branched Alkanes and Substituted Branched Alkanes

“What is the IUPAC name for the following compound?”

This is a simple alkyl-substituted alkane that helps students work through prefixes and identifying the longest chain.

A.6. Ethers and Alkoxy Groups

“What is the IUPAC name for the following ether?”

This problem combines a cyclic (cyclopentane) with two methyl groups and a methyl ether, which is a nice combination of groups that students often find challenging but that become easy after a classroom explanation.