CHAPTER

BOND-LINE DRAWINGS

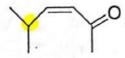
To do well in organic chemistry, you must first learn to interpret the drawings that organic chemists use. When you see a drawing of a molecule, it is absolutely critical that you can read all of the information contained in that drawing. Without this skill, it will be impossible to master even the most basic reactions and concepts.

Molecules can be drawn in many ways:



Cordansed or

(CH₃)₂CHCH=CHCOCH₃



Structural

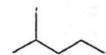
Without a doubt, the last structure (bond-line drawing) is the quickest to draw, the quickest to read, and the best way to communicate. Open your textbook to any page in the second half and you will find that every page is plastered with bond-line drawings. Most students will gain a familiarity with these drawings over time, not realizing how absolutely critical it is to be able to read these drawings fluently. This chapter will help you develop your skills in reading these drawings quickly and fluently.

1.1 HOW TO READ BOND-LINE DRAWINGS

Bond-line drawings show the carbon skeleton (the connections of all the carbon atoms that build up the backbone, or skeleton, of the molecule) with any functional groups that are attached, such as -OH or -Br. Lines are drawn in a zigzag format, so that the end of every line represents a carbon atom. For example, the following compound has 6 carbon atoms:



It is a common mistake to forget that the ends of lines represent carbon atoms as well. For example, the following molecule has six carbon atoms (make sure you can count them):



Double bonds are shown with two lines, and triple bonds are shown with three

etry). This can be quite confusing at first, because it can get hard to see just how many carbon atoms are in a triple bond, so let's make it clear: because triple bonds are linear (there will be more about this in the chapter on geom-When drawing triple bonds, be sure to draw them in a straight line rather than zigzag, 5,09

is the same as

6 carbon atoms so this compound has

two carbons connected to them are drawn in a straight line. All other bonds are Don't let triple bonds confuse you. The two carbon atoms of the triple bond and the drawn as a zigzag:

is drawn like this:

is drawn like this:

drawings: EXERCISE 1.1 Count the number of carbon atoms in each of the following

five carbon atoms: Answer The first compound has six carbon atoms, and the second compound has

drawings. PROBLEMS Count the number of carbon atoms in each of the following

> 1.6 1.2 Answer: Answer: 1.10 1.7 1.3 Answer: Answer: Answer: 1.11 Answer:_ 1.8 1.4 Answer: Answer: 1.9 .5 Answer: Answer:

neutral carbon atoms always have a total of four bonds. In the following drawing, the rule for determining how many hydrogen atoms there are on each carbon atom; the highlighted carbon atom is showing only two bonds: not shown, and this is why it is so easy and fast to draw bond-line drawings. Here is the hydrogen atoms in a bond-line drawing of a molecule. The hydrogen atoms are Now that we know how to count carbon atoms, we must learn how to count

connected to this carbon atom We see only two bonds

of hydrogen atoms even though they are not shown. son knows how to count to four, and therefore is capable of determining the number to save so much time when drawing molecules. It is assumed that the average pertotal of four bonds). This is what allows us to avoid drawing the hydrogen atoms and Therefore, it is assumed that there are two more bonds to hydrogen atoms (to give a

atoms without counting them. Now we will do some exercises that will help you get these types of drawings, and you will be able to instantly "see" all of the hydrogen where you do not need to count anymore. You will simply get accustomed to seeing of four bonds to the carbon atom. After doing this many times, you will get to a point atom, and then you know that there should be enough hydrogen atoms to give a total So you only need to count the number of bonds that you can see on a carbon

ber of hydrogen atoms connected to each carbon atoms. Count the num-

PROBLEMS For each of the following molecules, count the number of hydrogen atoms connected to each carbon atom. The first problem has been solved for you (the numbers indicate how many hydrogen atoms are attached to each carbon).

Now we can understand why we save so much time by using bond-line drawings. Of course, we save time by not drawing every C and H. But, there is an even larger benefit to using these drawings. Not only are they easier to draw, but they are easier to read as well. Take the following reaction for example:

It is somewhat difficult to see what is happening in the reaction. You need to stare at it for a while to see the change that took place. However, when we redraw the reaction using bond-line drawings, the reaction becomes very easy to read immediately:

As soon as you see the reaction, you immediately know what is happening. In this reaction we are converting a double bond into a single bond by adding two hydrogen atoms across the double bond. Once you get comfortable reading these drawings, you will be better equipped to see the changes taking place in reactions.

1.2 HOW TO DRAW BOND-LINE DRAWINGS

Now that we know how to read these drawings, we need to learn how to draw them. Take the following molecule as an example:

To draw this as a bond-line drawing, we focus on the carbon skeleton, making sure to draw any atoms other than C and H. All atoms other than carbon and hydrogen must be drawn. So the example above would look like this:

A few pointers may be helpful before you do some problems.

1. Don't forget that carbon atoms in a straight chain are drawn in a zigzag format:

is drawn like this:

2. When drawing double bonds, try to draw the other bonds as far away from the double bond as possible:

is much better than

3. When drawing zigzags, it does not matter in which direction you start drawing:

is the same as

is the same as

PROBLEMS For each structure below, draw the bond-line drawing in the box

1.21

1.22

1.23

(CH₃)3C-C(CH₃)3

11

1.3

1.24

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1.3 MISTAKES TO AVOID

- MISTAKES TO AVOID
- When drawing a molecule, you should either show all of the H's and all of orbitals of another atom). This is true of all second-row elements, and we Never draw a carbon atom with more than four bonds. This is a big no-no. discuss this in more detail in the chapter on drawing resonance structures. only four bonds (bonds are formed when orbitals of one atom overlap with Carbon atoms only have four orbitals; therefore, carbon atoms can form

C-C-C-C C Never do this

the C's, or draw a bond-line drawing where the C's and H's are not drawn.

You cannot draw the C's without also drawing the H's:

put in the H's: This drawing is no good. Either leave out the C's (which is preferable) or

9 I-0

3. When drawing each carbon atom in a zigzag, try to draw all of the bonds as far apart as possible:

other than carbon. For example

4. In bond-line drawings, we do draw any H's that are connected to atoms

is better than

The state of the s

.4 MORE EXERCISES

First, open your textbook and flip through the pages in the second half. Choose any bond-line drawing and make sure that you can say with confidence how many carbon atoms you see and how many hydrogen atoms are attached to each of those carbon atoms.

Now try to look at the following reaction and determine what changes took place:

Do not worry about *how* the changes took place. You will understand that later when you learn the mechanism of the reaction. For now, just focus on explaining what change took place. For the example above, we can say that we *added* two hydrogen atoms to the molecule (one on either end of the double bond).

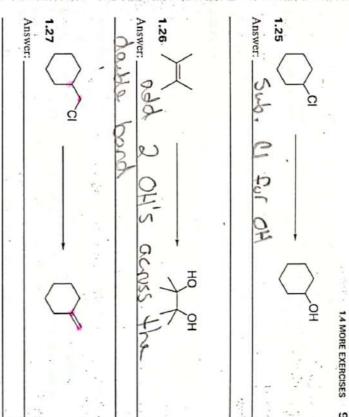
Consider another example:

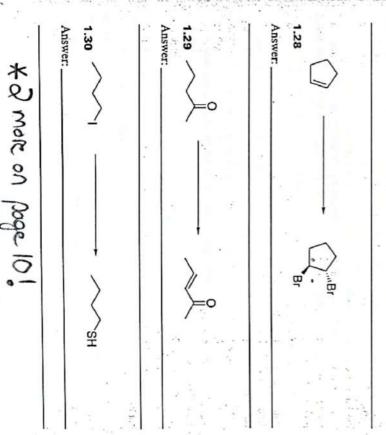
In this example, we have eliminated an H and a Br to form a double bond. (We will see later that it is actually H⁺ and Br⁻ that are eliminated, when we get into the chapters on mechanisms). If you cannot see that an H was eliminated, then you will need to count the number of hydrogen atoms in the starting material and compare it with the product:

Now consider one more example:

In this example, we have substituted a bromine with a chlorine.

PROBLEMS For each of the following reactions, clearly state what change has taken place. In each case your sentence should start with one of the following opening clauses: we have added . . . , we have climinated . . . , or we have substituted



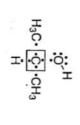


1.5 IDENTIFYING FORMAL CHARGES 11

Remember that every bond represents two electrons being shared between two atoms. Begin by splitting each bond apart, placing one electron on this atom and one electron on that atom:



atom: Now count the number of electrons immediately surrounding the central carbon



There are four electrons. This is the number of electrons that the atom actually has.

cases, there will be a formal charge. So let's see an example of an atom that has a to have and the number of electrons the atom actually has will be different. In those draw in this course. But in some cases, the number of electrons the atom is supposed mal charge. This will be the case for most of the atoms in the structures you will supposed to have (in this case, four) with how many valence electrons it actually has formal charge. (in this case, four). Since these numbers are the same, the carbon atom has no for-Now we are in a position to compare how many valence electrons the atom is

Consider the oxygen atom in the structure below: actually has 7 e-

Supposed to have 6 e-

ting up the C-O bond: valence electrons. Next, we need to look at the oxygen atom in this compound and have. Oxygen is in the sixth column of the periodic table, so oxygen should have six ask how many valence electrons it actually has. So, we redraw the molecule by split-Let's begin by asking how many valence electrons oxygen atoms are supposed to *will have -1 charge



to form a bond. Lone pairs are drawn as two dots on an atom, and the oxygen above has three of these lone pairs. You must remember to count each lone pair as two three lone pairs. A lone pair is when you have two electrons that are not being used In addition to the electron on the oxygen from the C-O bond, the oxygen also has

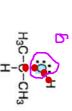
1.32 Answer: Answer: 10 CHAPTER 1 BOND-LINE DRAWINGS IDENTIFYING FORMAL CHARGES

atom is supposed to have. has four valence electrons. Now you know how to determine how many electrons the us how many valence electrons there are (valence electrons are the electrons in the high school chemistry). For example, carbon is in the fourth column, and therefore valence shell, or the outermost shell of electrons—you probably remember this from from the periodic table. The column of the periodic table that the atom is in will tell number of valence electrons the atom is supposed to have. We can get this number do we calculate formal charges? hard time passing this course. them. If you cannot do this, then you will not be able to draw resonance structures So you must learn how to identify when you need formal charges and how to draw formal charges. By doing this, you will understand what formal charges are. So how (which we see in the next chapter), and if you can't do that, then you will have a very When calculating the formal charge on an atom, we first need to know the To understand what formal charges are, we begin by learning how to calculate

when it is supposed to be drawn, then your drawing will be incomplete (and wrong). on our drawings. They are extremely important. If you don't draw a formal charge Formal charges are charges (either positive or negative) that we must often include

Next we look in our drawing and ask how many electrons the atom actually

has in the drawing. But how do we count this? Let's see an example. Consider the central carbon atom in the compound



"one" valence electron Count each bond as

electron than it is supposed to have. Therefore, it will have a negative charge: electrons. So we see that the oxygen actually has seven electrons, which is one more

mine if it has a formal charge: EXERCISE 1.33 Consider the nitrogen atom in the compound below and deter-

should have 5 esee it with 4 e-

missing 1 e = + charge

Answer Nitrogen is in the fifth column of the periodic table so it should have five electrons. Now we count how many it actually has:

your head Sep. the electrons in

this nitrogen atom has a positive charge: It only has four. So, it has one less electron than it is supposed to have. Therefore,

on the structure gen atom in the molecule has a formal charge. If there is a charge, draw the charge PROBLEMS For each of the compounds below determine if the oxygen or nitro-

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1.5 IDENTIFYING FORMAL CHARGES

3

1.42 drawing bond-line structures, because it is assumed that we know how to count to carbon always has four bonds. This allows us to ignore the hydrogen atoms when This brings us to the most important atom of all: carbon. We saw before that 1.44

then we will move on to C-. four bonds. In fact, it will have only three. Let's see why. Let's first consider C+, and formal charge is, let's consider what happens when carbon has a formal charge. If carbon bears a formal charge, then we cannot just assume the carbon has

most structures will not have formal charges). But now that we have learned what a were only talking about carbon atoms without formal charges (most carbon atoms in

four and can figure out how many hydrogen atoms are there. When we said that, we

should count hydrogen atoms with this in mind: odic table). Since it has only three electrons, it can form only three bonds. That's it supposed to have four electrons, because carbon is in the fourth column of the peri-So, a carbon with a positive formal charge will have only three bonds, and you If carbon has a positive formal charge, then it has only three electrons (it is

No hydrogen atoms on this C+

I hydrogen atom on this C+

2 hydrogen atoms on this C+

electrons form a lone pair, and the other three electrons are used to form bonds: electron than it is supposed to have. Therefore, it has five electrons. Two of these mal charge. The reason it has a negative formal charge is because it has one more Now let's consider what happens when we have a carbon with a negative for-

with a negative charge will have a lone pair (if you look at the drawing above, you space called orbitals. These orbitals can overlap with orbitals from other atoms to a bond. Carbon can never have five bonds. Why not? Electrons exist in regions of will count four orbitals—one for the lone pair and then three more for the bonds). it does not have five orbitals to use to form those bonds. This is why a carbon atom form bonds, or the orbitals can contain two electrons (which is called a lone pair) Carbon has only four orbitals, so there is no way it could possibly form five bonds— We have the lone pair, because we can't use each of the five electrons to form

Therefore, a carbon atom with a negative charge can also form only three bonds (just like a carbon with a positive charge). When you count hydrogen atoms, you should keep this in mind:

To hydrogen atoms on this

No hydrogen atoms on this C

1.6 FINDING LONE PAIRS THAT ARE NOT DRAWN

From all of the cases above (oxygen, nitrogen, carbon), you can see why you have to know how many lone pairs there are to figure out the formal charge on an atom. Similarly, you have to know the formal charge to figure out how many lone pairs there are on an atom. Take the case below with the nitrogen atom shown:

If the lone pairs were drawn, then we would be able to figure out the charge (two lone pairs would mean a negative charge and one lone pair would mean a positive charge). Similarly, if the formal charge was drawn, we would be able to figure out how many lone pairs there are (a negative charge would mean two lone pairs and a positive charge would mean one lone pair).

So you can see that drawings must include either lone pairs or formal charges. The convention is to always show formal charges and to leave out the lone pairs. This is much easier to draw, because you usually won't have more than one charge on a drawing (if even that), so you get to save time by not drawing every lone pair on every atom.

Now that we have established that formal charges must always be drawn and that lone pairs are usually not drawn, we need to get practice in how to see the lone pairs when they are not drawn. This is not much different from training yourself to see all the hydrogen atoms in a bond-line drawing even though they are not drawn. If you know how to count, then you should be able to figure out how many lone pairs are on an atom where the lone pairs are not drawn.

Let's see an example to demonstrate how you do this:

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In this case, we are looking at an oxygen atom. Oxygen is in the sixth column of the periodic table, so it is supposed to have six electrons. Then, we need to take the formal charge into account. This oxygen atom has a negative charge, which means one extra electron. Therefore, this oxygen atom must have 6+1=7 electrons. Now we can figure out how many lone pairs there are.

The oxygen has one bond, which means that it is using one of its seven electrons to form a bond. The other six must be in lone pairs. Since each lone pair is two electrons, this must mean that there are three lone pairs:

o is the same as

Let's review the process:

- Count the number of electrons the atom should have according to the periodic table.
- Take the formal charge into account. A negative charge means one more electron, and a positive charge means one less electron.
- Now you know the number of electrons the atom actually has. Use this number to figure out how many lone pairs there are.

Now we need to get used to the common examples. Although it is important that you know how to count and determine numbers of lone pairs, it is actually much more important to get to a point where you don't have to waste time counting. You need to get familiar with the common situations you will encounter. Let's go through them methodically.

When oxygen has no formal charge, it will have two bonds and two lone pairs:

If oxygen has a negative formal charge, then it must have one bond and three lone pairs:

If oxygen has a positive charge, then it must have three bonds and one lone pair:

EXERCISE 1.46 Draw in all lone pairs in the following structure:

Answer The oxygen has a positive formal charge and three bonds. You should try to get to a point where you recognize that this must mean that the oxygen has one lone pair:

Until you get to the point where you can recognize this, you should be able to figure out the answer by counting.

Oxygen is supposed to have six electrons. This oxygen atom has a positive charge, which means it is missing an electron. Therefore, this oxygen atom must have 6-1=5 electrons. Now, we can figure out how many lone pairs there are.

The oxygen has three bonds, which means that it is using three of its five electrons to form bonds. The other two must be in a lone pair. So there is only one lone pair.

PROBLEMS Review the common situations above, and then come back to these

problems. For each of the following structures, draw in all lone pairs. Try to recognize how many lone pairs there are without having to count. Then count to see if you were right.

1.47

Now let's look at the common situations for nitrogen atoms. When nitrogen has no formal charge, it will have three bonds and one lone pair:

If nitrogen has a negative formal charge, then it must have two bonds and two lone pairs:

is the same as

If nitrogen has a positive charge, then it must have four bonds and no lone pairs:

has no lone pairs

(remember from the previous section that C+ has no lone pairs and C- has one lone MORE PROBLEMS For each of the following structures, draw in all lone pairs

EXERCISE 1.53 Draw all lone pairs in the following structure:

try to get to a point where you recognize that this must mean that this nitrogen has no lone pairs. The bottom nitrogen has no formal charge and three bonds. You should try to get to a point where you recognize that this must mean that this nitrogen has Answer The top nitrogen has a positive formal charge and four bonds. You should one lone pair:

electrons to form bonds. So there is no lone pair on this nitrogen atom. trogen atom has a positive charge, which means it is missing an electron. This means out the answer by counting. Nitrogen is supposed to have five electrons. The top ni-Until you get to the point where you can recognize this, you should be able to figure many lone pairs there are. Since this nitrogen has four bonds, it is using all of its that this nitrogen atom must have 5-1=4 electrons. Now we can figure out how

recognize how many lone pairs there are without having to count. Then count to see these problems. For each of the following structures, draw in all lone pairs. Try to electrons. It has three bonds, which means that there are two electrons left over, and PROBLEMS Review the common situations for nitrogen, and then come back to they form a lone pair. The bottom nitrogen atom has no formal charge, so this nitrogen atom has five

if you were right.

1.57

1.61 .62