# Chapter 2. Bonding and Structure

2.1 Electron waves

The world really is strange. It is stranger than most people realize. Back in your Junior High Science class, you were probably told about the duality of light, where light is both a particle and a wave. This wave/particle duality is not only true about light, but it is true about most of nature. This is the strangeness that we explore in a field called quantum mechanics.

For now, I want us to focus on the wave/particle duality of electrons. One way to think about electrons is that they are little particles orbiting the nucleus. This is a fairly good model that many of us have in our minds, the Bohr planetary model. But, the interesting thing is that electrons are also waves! Let's focus on two very simple waves. Think of a guitar string. If I pluck a guitar string, it vibrates up and down.
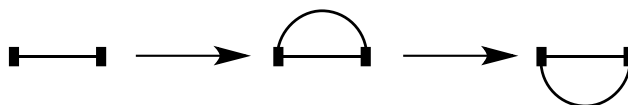
If I combine these, the string vibrates so fast that it looks something like this.
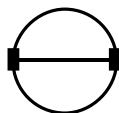
This simple vibrational shape is spherical in nature and leads us to the shape of the simplest electron orbital, the s orbital.
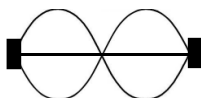
Figure 2.1 The s orbital

If I put my finger down in the middle of the guitar string and pluck it, I get a wave where when one side is up, the other side is down. A moment later, it switches which side is up and which is down.
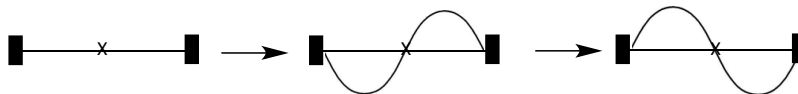
When the string vibrates fast, it looks something like this.

There is one spot in the center where there is no wave. We say that it has one node in the center. This vibrational shape has two lobes of equal size. It leads us to the shape of another electron orbital, the p orbital.
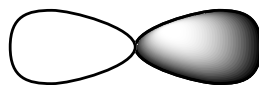
Figure 2.2 The p orbital

These orbital waves can be described with mathematical functions—just like all waves can. We call this mathematical function for the wave the wavefunction which is often represented by the greek letter psi (**Ψ**). These mathematical functions can be added together or subtracted. Intuitively, you understand this about waves.

Photo by GaborfromHungary at Morguefile.com

For example, a child on a swing set moves forward and backward. This motion is a wave-like motion. When children are learning to swing on a swing set, they are taught to kick their legs out when they are moving forward and bend at the knees and put their feet down when they are moving backward. This motion of their feet is also a wave. They are taught to do this so that their feet wavefunction can be added to the wavefunction of the swing. *Constructive interference* is when two waves overlap to make a larger wave. When done correctly, the child's feet motion and the swinging motion constructively interfere to increase the amplitude of the wave, and their swinging, so they go higher and higher.

Many children get confused when learning this, though. If instead, they kicked their feet straight out when they were going backward and bent their knees putting their feet down when they were going forward, their feet wave would be opposite the swing's wave. *Destructive interference* is when two waves are out of phase with each other making smaller waves. Children who swing this way will not be swinging for long. When the wavefunctions destructively interfere, they are subtracted from each other and get canceled out.

Two electron orbitals can add constructively or destructively because they are waves. This can happen when orbitals overlap on the same atom (to make hybrid orbitals) or when orbitals on two different atoms overlap when the atoms come close together (to make molecular orbitals or bonds).

2.2 Atomic orbitals

A hydrogen atom (atomic number 1) has only one electron surrounding one positive proton in the nucleus. This lone electron is in a round orbital called a 1s orbital and is in the first and only shell of electrons of the hydrogen atom. The outermost electrons of an atom are called its valence electrons. Since this first shell is also the outermost shell of electrons, this 1s electron is the *only* valence electron for hydrogen.

Figure 2.3 Hydrogen atom, one shell, 1s orbital

The first shell is small and can only hold two electrons in it. Helium (atomic number 2) fills up this first shell with its two electrons, both in the 1s orbital. Another shell of electrons outside of this first shell is needed for the other important organic chemistry atoms like carbon, nitrogen and oxygen because they contain more than two electrons. Therefore, these other important organic chemistry atoms have two shells of electrons.
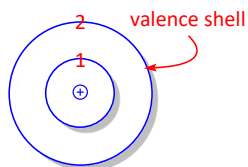
Figure 2.4 The two electron shells of common organic atoms

For these atoms, the first, innermost shell of electrons is made up of two electrons in a round orbital called a 1s orbital. These two electrons are not very interesting because they are tucked inside the atom and don't interact with other atoms. The second shell is farther away from the positively charged nucleus. It is more interesting because it contains the outermost electrons of the atom. These electrons are the ones that will bump into other atoms to form bonds. This outermost electron shell is called the valence shell and its electrons are the valence electrons. It is also made up of two electrons in a round orbital called a 2s orbital. It is the same shape as the 1s orbital, but just a little bigger as the electrons are a little farther from the nucleus in the second shell.

1s   2s
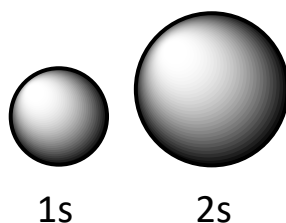
The round 2s orbital is not the only type of electron orbital in the 2nd shell. There are also three double-lobed 2p orbitals in this valence shell. These three p orbitals are all rotated 90° from each other.
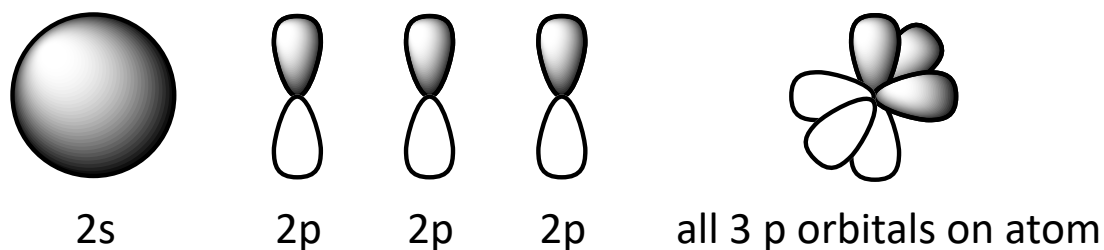

2s   2p   2p   2p   all 3 p orbitals on atom

Figure 2.5 Atomic orbitals

They all have the number "2" in them because they make up the second shell – that is, the meatiest parts of these orbitals are all about the same distance away from the nucleus, where the 2nd shell is located.
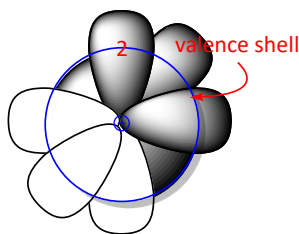

Figure 2.6 Showing how 2s and 2p orbitals make the valence (2nd) shell

This is what the atomic orbitals of carbon atom look like. To make bonds between atoms, the outermost valence electrons of one atom must overlap with the outermost valence electrons of another atom to make bonds. If the atomic orbitals described above were the only electron orbitals that atoms contain, we would expect that we could only bond atoms with a carbon atom at 90° and 180° angles. This is not the case. We often see bond angles of 180°, 120°, and 109.5°, but not 90°. Let's look at methane (CH_4) if only atomic orbitals can overlap compared to its true, tetrahedral shape.
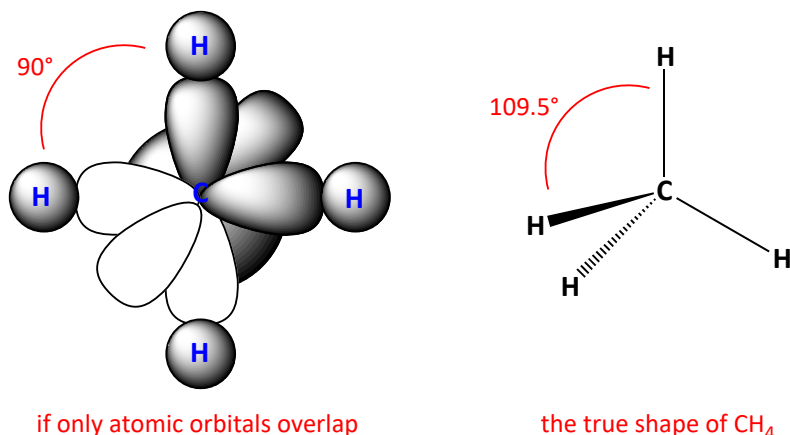

if only atomic orbitals overlap   the true shape of CH_4

Figure 2.7 CH_4 if only atomic orbitals overlap vs. its true shape

Something else must be going on to get these other bond angles. Because all electron orbitals are waves, we can get these other bonding angles when the s and p atomic orbitals that are on the same atom mix together to form new oblong electron orbitals that are called *hybrid orbitals*. A hybrid is the offspring of two different species. So hybrid orbitals are the offspring of two different types of orbitals on the same atom. It is important that you realize we are mixing together electron waves on *the same* atom because mixing together orbitals that are on *different* atoms is something else entirely, something we call making bonds.

2.3 Hybrid orbitals

What are they?

This is how we mix atomic orbitals on the same atom together to make hybrid orbitals. We mix together the outside, valence electrons. The number of atomic orbitals that mix together is the exact same number of hybrid orbitals that are created, always. So, if two atomic orbitals (2s and 2p) are mixed together, that will make two hybrid orbitals. Those hybrid orbitals would be called sp hybrid orbitals because they are made from one s and one p orbital. If three atomic orbitals (2s, 2p, 2p) are mixed together, that will make three hybrid orbitals. Those hybrid orbitals would be called sp^2 hybrid orbitals because they are made from one s and two p orbitals. If four atom orbitals (2s, 2p, 2p, 2p) are mixed together, that will make four hybrid orbitals. Those hybrid orbitals would be called sp^3 hybrid orbitals because they are made from one s and three p orbitals.

Their shapes

Like charges repel each other. Since these hybrid orbitals all contain negative electrons, they repel each other. This means the hybrid orbitals that are formed get as far away from each other as possible. If all four valence atomic orbitals (2s, 2p, 2p, 2p) are mixed, four sp^3 hybrid orbitals are made. When these four orbitals get as far away from each other as they can, they form a tetrahedral shape with an angle of 109.5° between them. This is what happened in our methane, CH_4, example earlier. If three of the four valence atomic orbitals are mixed (2s, 2p, 2p), then three sp^2 hybrid orbitals are made. When these three orbitals try to get as far away from each other as they can, they form a trigonal planar shape with an angle of 120° between them. If only two of the four

valence atomic orbitals mix (2s, 2p) then two sp hybrid orbitals are made. When these two hybrid orbitals try to get as far away from each other as they can, they form a linear shape with an angle of 180° between them.
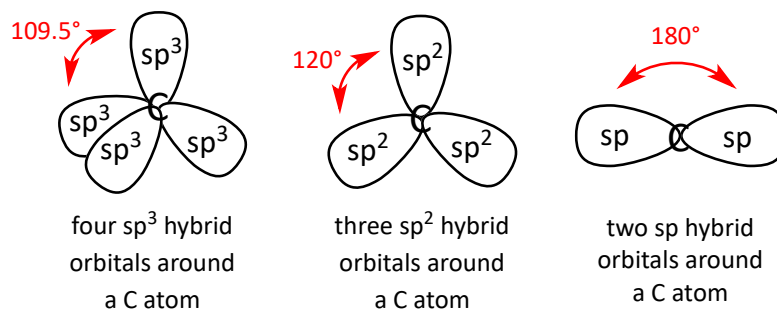
Figure 2.8 Geometry of hybrid orbitals

The unhybridized p orbitals

We are almost there, but this is not the complete picture. Most of the important organic chemistry atoms (outside of hydrogen) start with one s and three p valence atomic orbitals—four total. So, if we start with four atomic orbitals, we must end up with four total orbitals in the end, always. We must not forget about the atomic orbitals that are *not* mixed together to make the hybrids. When we make sp^2 hybrid orbitals, we mix three out of the four orbitals, the s, and two p orbitals to make three sp^2 hybrid orbitals. There is a p atomic orbital left over, untouched, that is not mixed at all! It is unchanged. We call it an unhybridized orbital because, well, it's not hybridized. It is still on the atom as a regular old p orbital. When we make sp hybrid orbitals, we mix two out of the four atomic orbital, the s and p to make two sp hybrid orbitals. There are two p orbitals that remain untouched or unhybridized.
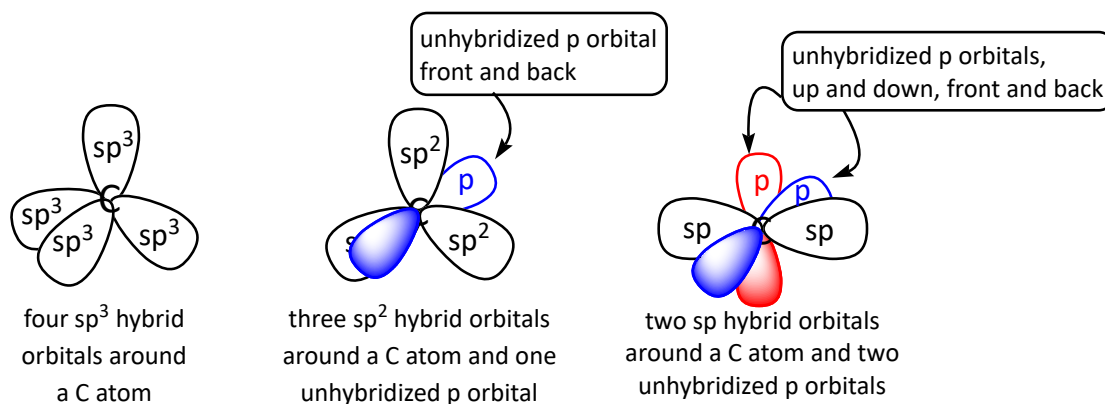
Figure 2.9 The unhybridized p orbitals with hybrid orbitals

2.3.2 What is the hybridization of an atom?

How does one determine what the hybridization (sp, sp^2, or sp^3) is for an atom? You need to count how many electron groups are on the atom. Lone pairs of electrons, even though they don't point to an atom, count as electron groups since they do take up space. They must be in a hybrid orbital. Additionally, single bonds, double bonds and triple bonds each count as only one electron group since they each point to one atom. Alternatively, you can count the atoms at the ends of those single, double, or triple bonds.

We can determine the hybridization for an atom after we have counted the number of electron groups on it. If *two* electron groups are on an atom, it needs two hybrid orbitals – one for each electron group. Such an atom

has sp hybridization because sp hybridization is when one s and one p orbital overlap to make *two* sp hybrid orbitals. If *three* electron groups are on an atom, it needs three hybrid orbitals. Such an atom has sp^2 hybridization because sp^2 hybridization is when one s and two p atomic orbitals mix to make *three* sp^2 hybrid orbitals. If *four* electron groups are on an atom, the atom has sp^3 hybridization because sp^3 hybridization is when one s and three p atomic orbitals mix to make *four* sp^3 hybrid orbitals.

Let's look at an example, the hybridization of the carbon and oxygen atoms of formaldehyde. Let's analyze the oxygen atom first. We notice that the oxygen atom has two lone pairs of electrons (1 and 2). We always need to remember that electron pairs take up space and need to go into a hybrid orbital. The oxygen atom also has one atom attached (the carbon on the double bond labeled 3). This is a total of three electron groups, so the oxygen atom needs three hybrid orbitals. It is therefore sp^2 hybridized (one s and two p orbitals gives three sp^2 hybrid orbitals). When we analyze the carbon atom's hybridization, we notice there are no electron pairs of electrons on the carbon, but there are three atoms attached to it. These three atoms are the oxygen atom at the end of the double bond (1) and the two hydrogen atoms (2 and 3). With three electron groups on the carbon atom, it is also sp^2 hybridized.
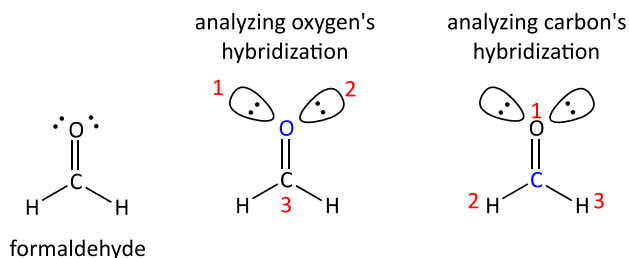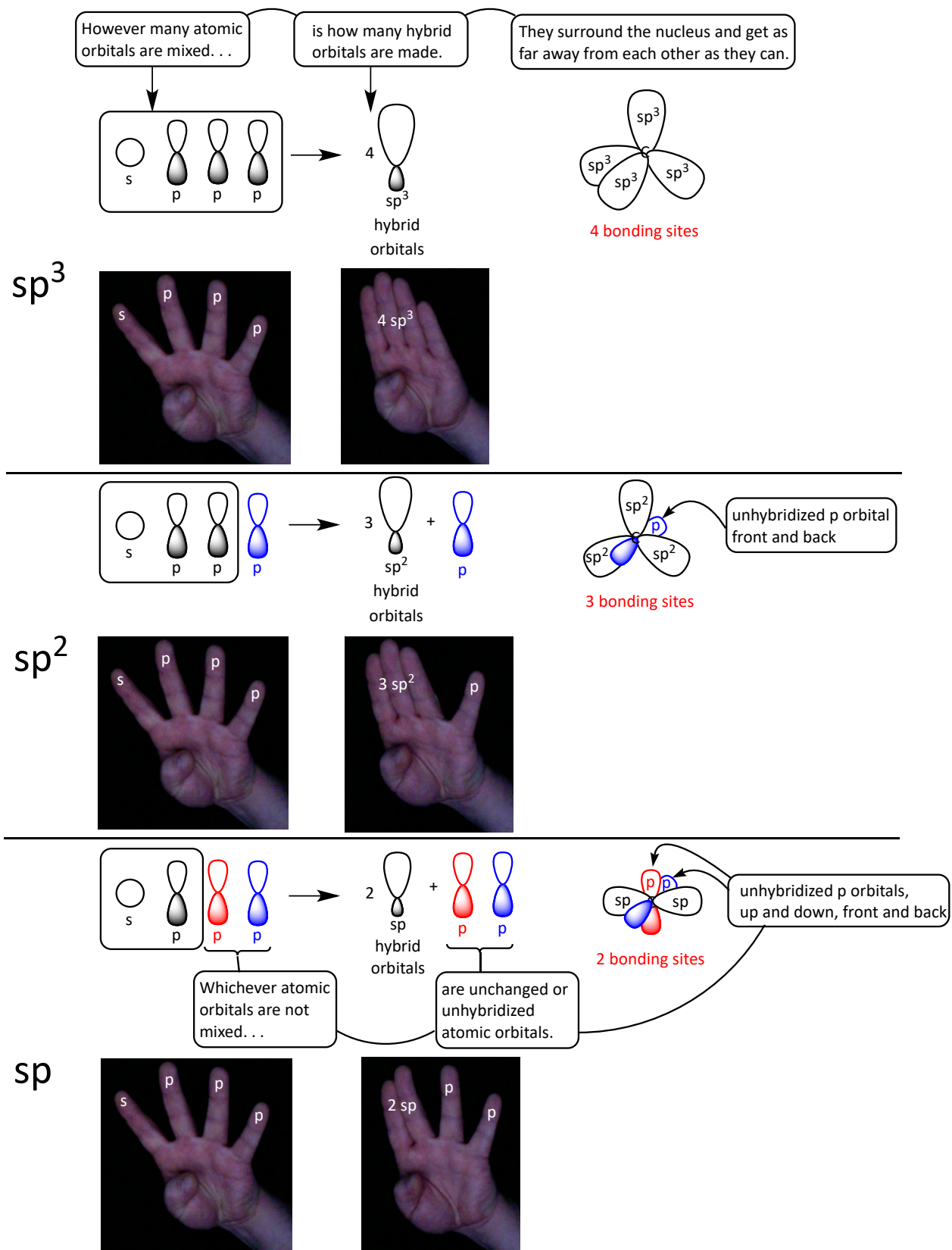

Figure 2.10 Hybridization of atoms in formaldehyde

However many atomic orbitals are mixed. . .

is how many hybrid orbitals are made.

They surround the nucleus and get as far away from each other as they can.

s p p p

$\rightarrow$ 4 sp^3 hybrid orbitals

sp^3 sp^3 sp^3 sp^3

4 bonding sites

sp^3

s p p p

4 sp^3

---

s p p p

$\rightarrow$ 3 sp^2 hybrid orbitals + p

sp^2 sp^2 sp^2 p

unhybridized p orbital front and back

3 bonding sites

sp^2

s p p p

3 sp^2 p

---

s p p p

$\rightarrow$ 2 sp hybrid orbitals + p p

sp p p sp

unhybridized p orbitals, up and down, front and back

2 bonding sites

Whichever atomic orbitals are not mixed. . .

are unchanged or unhybridized atomic orbitals.

sp

s p p p

2 sp p p

Figure 2.11 Hybrid orbitals

2.3.3 Hybridization of atoms in some common bonding patterns

For neutral carbon atoms in most organic chemistry molecules, if it contains only single bonds, it is sp^3 hybridized. If a carbon atom contains one double bond, it is sp^2 hybridized. If a carbon atom contains one triple bond, it is sp hybridized. Below are common hybridizations and show how to count the electron groups.

sp

Count the two electron groups on each atom

2 atoms
0 lone pairs

2 atoms
0 lone pairs

sp^2

Count the three electron groups on each atom

3 atoms
0 lone pairs

1 atom
2 lone pairs

2 atoms
1 lone pair

3 atoms
0 lone pairs

sp^3

Count the four electron groups on each atom

4 atoms
0 lone pairs

1 atom
3 lone pairs
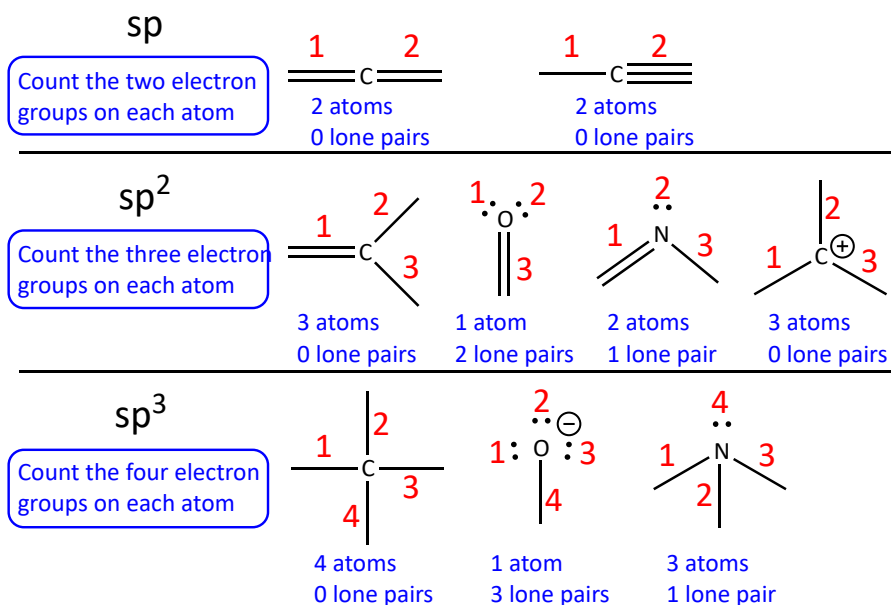
3 atoms
1 lone pair

Figure 2.12 Common hybridization bonding patterns

2.1 Identify the hybridization on the central atoms of the amino acid, histidine.

Histidine
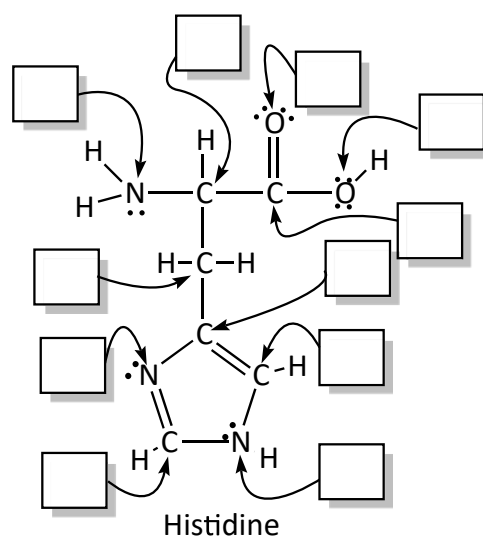
2.4 Molecular orbitals

2.4.1 Sigma and Pi Bonds

When two atoms come together, the electron orbitals on the atoms can overlap. This constructive overlap of electron density between two atoms makes bonding molecular orbitals, also called bonds. There are two main types of bonds we will deal with in organic chemistry, sigma and pi bonds. A sigma bond is directly between two atomic nuclei. Or, a more technical way to describe it is the electron density lies on the internuclear axis. A pi bond has electron density above and below the internuclear axis.
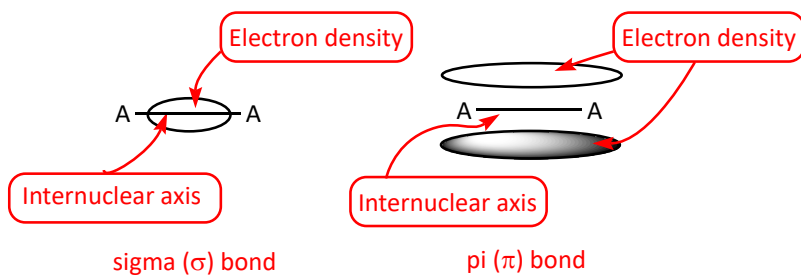
Figure 2.13 Sigma and pi-bonds

A mnemonic to help you learn these at first is to think of the first, single bond between two atoms as a snake, the sigma snake. This can help you think of a sigma bond. The second bond is split into two regions, above and below the internuclear axis. A pi bond may remind you of a *pie* crust.
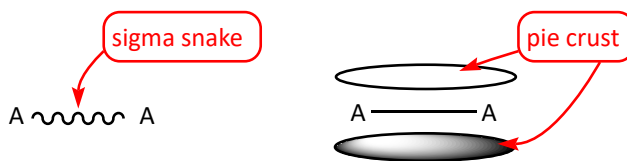
Figure 2.14 Sigma and pi-bond mnemonics

We've learned that hybridization is a mixing of atomic orbitals on one atom. We need to look at how two or more atoms come together to make bonds and form molecules. We mix hybrid and/or atomic orbitals to make these molecular orbitals. These bonds that we form between atoms are called molecular bonds.

Atomic orbitals are s and p orbitals on individual atoms.

Hybrid orbitals are sp, sp^2, s p^3 orbitals that are mixed from the s and p atomic orbitals <u>on the same atom</u>.

Molecular orbitals are a mixing of atomic and hybrid orbitals <u>between different atoms</u> to make bonds between those atoms. This is how we make molecules.

2.4.2 Alkane bonding

Let's look at how some simple molecules are put together. Let's begin with propane.

$$H_3C \text{---} CH_2 \text{---} CH_3$$
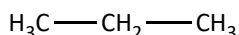
Let's redraw it in 3D. We see that each of the carbon atoms has four bonds and is sp^3 hybridized.
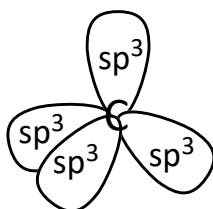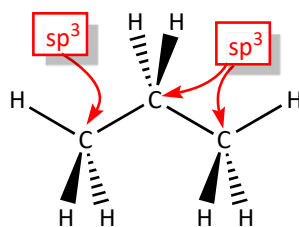
First, let's draw the central carbon atom with its four sp^3 hybrid orbitals around it. We draw it with the bottom two sp^3 hybrid orbitals pointing towards the bottom right and bottom left so they are pointing towards where the other carbon atoms will be drawn. Notice, when we draw the hybrid orbitals, we typically leave off the small back lobes on each one. This makes it easier to draw and makes it less complicated.

Now, let's draw the other, outside, carbon atoms with four sp^3 hybrid orbitals around each one.
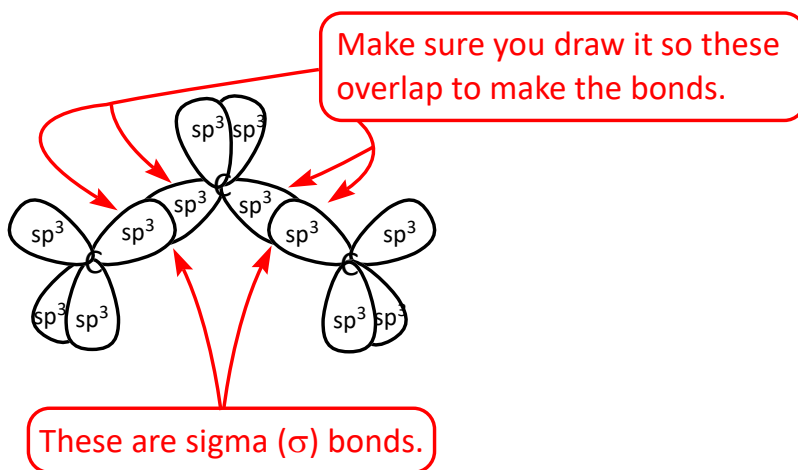
A sigma bond (σ-bond) is made by two hybrid orbitals overlapping directly between the nuclei of two atoms.

Finally, we draw in the hydrogen atoms. A hydrogen atom cannot make hybrid orbitals because it is just one 1s orbital. They are simple to draw. We draw the spherical 1s orbitals for each hydrogen atom. Notice, they overlap with the hybrid orbitals on the carbon atoms.
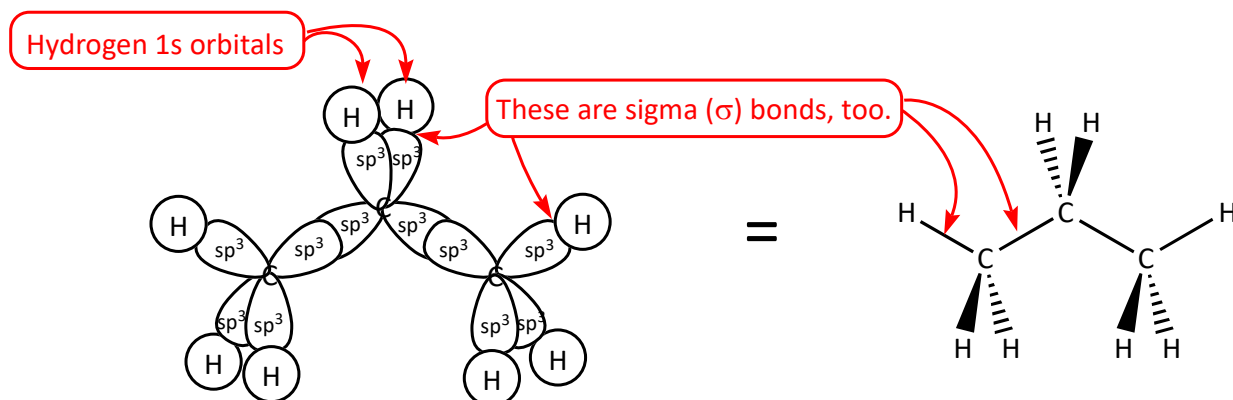
Figure 2.15 Orbital representation for propane

2.4.3 Alkene bonding

Let's look at something with a double bond in it, ethene.
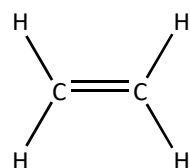
We identify the hybridization of the atoms.
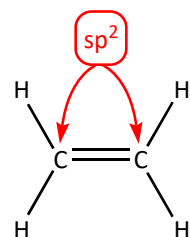
Then, we draw in the sp² hybrid orbitals around the carbon atoms making sure we arrange them so they overlap between the carbon atoms. If they do not overlap, they do not make a bond.
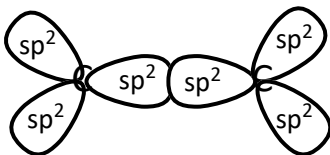
2.4.4 Pi bonds

But, whenever we have sp² hybridization, there is one atomic p-orbital on each carbon that remains unhybridized. If we draw those in, we see that they can overlap above and below the carbon-carbon internuclear axis. They make a pi bond (π-bond).
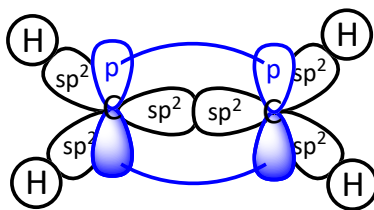
Notice, the σ-bond is the one that lies directly between the carbon nuclei. Notice the π-bond is above and below the internuclear axis (between the carbon nuclei). Half of the π-bond is above the plane and the other half is below the plane. These two parts together make one π-bond. So, there is one σ-bond and one π-bond between the carbon atoms. This is how we get a double bond. A double bond consists of one σ-bond and one π-bond.
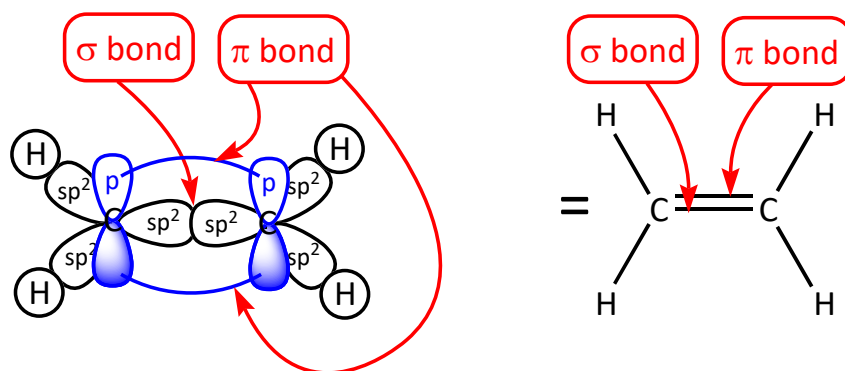
Figure 2.16 Orbital representation for ethene

2.4.5 Alkyne bonding

For acetylene, H-C≡C-H, the carbons are sp hybridized. There are two unhybridized p-orbitals on each carbon that can overlap to make two π-bonds.
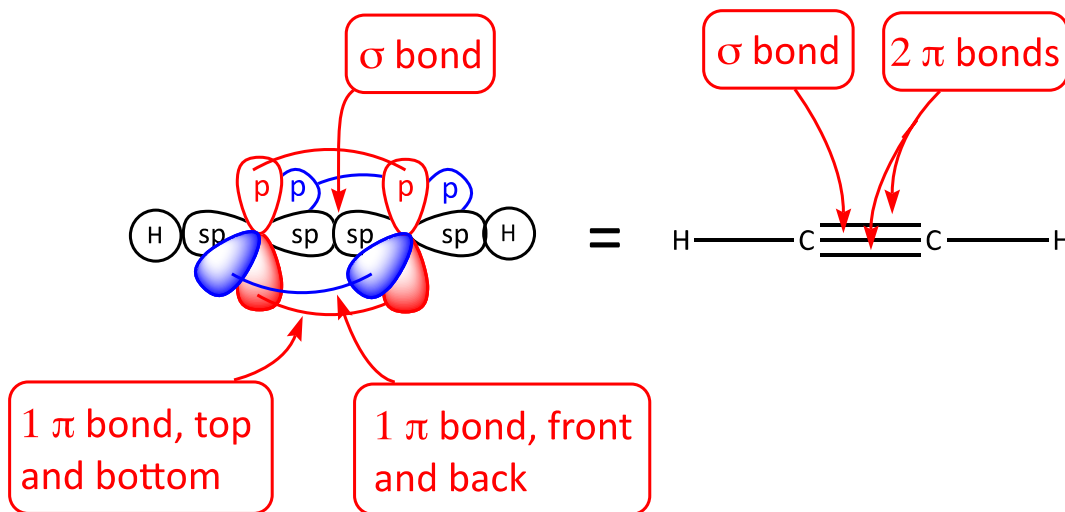
Figure 2.17 Orbital representation for ethyne

Important point

The first bond (the single bond) is a σ-bond. The second and third bonds of a multiple bond (double or triple bond) are π-bonds.

2.2 Identify the number of sigma bonds and pi bonds at the indicated bonding sites.

σ _____
π _____

σ _____
π _____

σ _____
π _____

σ _____
π _____

σ _____
π _____

σ _____
π _____
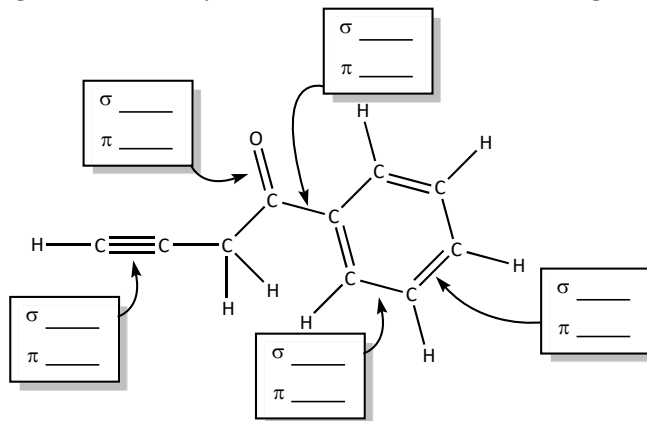
2.3 Draw an orbital representation for the cyanide ion, :C≡N:⁻.

2.5 Lewis Structures

Electrons. Chemistry is all about the electrons, those negative charges floating around on the outside of atoms. In fact, the most important electrons in chemistry are those that are on the very outside of the atom. That makes sense because when two atoms approach each other to react, those are the first ones that will bump into each other. These special, outside electrons are called "valence electrons." The number of valence electrons that surround an atom may be determined by its placement in the periodic table. Hydrogen has one valence electron, carbon has four, nitrogen and phosphorus have five, oxygen and sulfur have six, and the halogens have seven.

Figure 2.18 Periodic table column numbers showing the number of valence electrons

Bonding and Structure

The normal Lewis dot structures for these atoms have the valence electrons represented as dots around the atom. One electron is placed on each of the four sides of the atom before they are paired.

H•   •C•   •N•   •O•   :Cl•
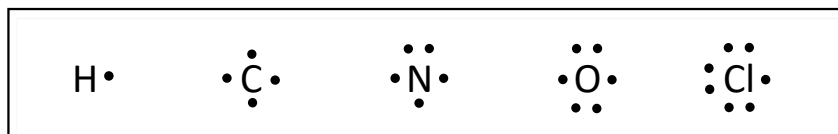
Figure 2.19 Valence electrons on organic chemistry elements

The normal bonding pattern for these atoms is with a bond at each site that has only one electron. It will be useful to know the normal bonding patterns of common atoms used in organic chemistry. This is important to aid us in drawing compounds as well as helping us recognize sites in molecules that may be the most reactive.

H•   •C•   •N•   •O•   :Cl•

H—   —C—   —N—   —O—   :Cl—
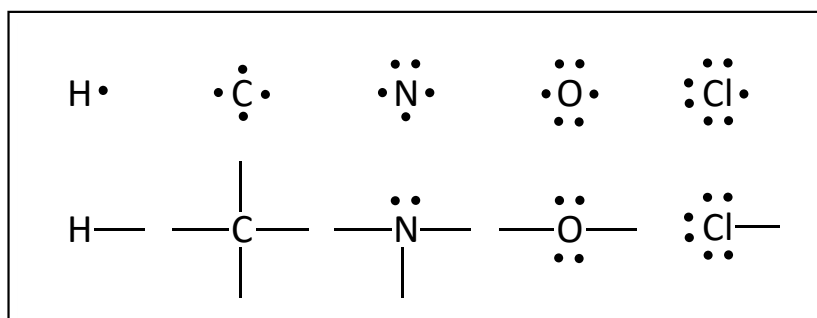
Figure 2.20 Number of bonds and lone pairs for organic chemistry atoms

Single bonds are not the only types of bonds you will see in organic chemistry. Double (=) and triple (≡) bonds are also commonly found. Because carbon, nitrogen, and oxygen normally form more than one bond, there is more than one normal bonding pattern for each of them.

1 bond 0 lone pairs	4 bonds 0 lone pairs	3 bonds 1 lone pair	2 bonds 2 lone pairs	1 bond 3 lone pairs
H—	—C—	—N—	—O—	:Cl—
	C=	N=	O (double bond)	
	—C≡	:N≡		
	=C=			
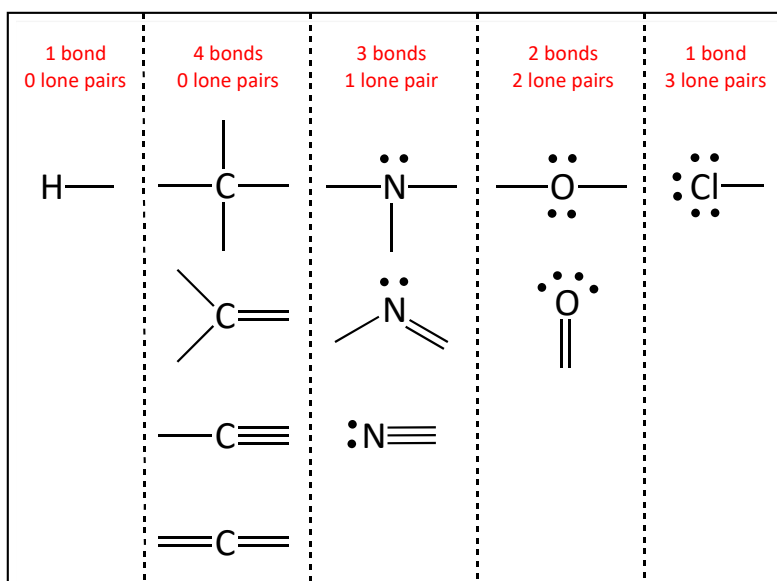
Figure 2.21 Common bonding patterns for organic chemistry atoms

24

There are four different bonding patterns for carbon. This is one of the reasons so many carbon-based, organic, compounds exist.

2.4 In each of the following compounds, the atoms are drawn, but the bonds and the lone pairs of electrons are missing. Using the normal bonding patterns for these atoms, fill in the bonds and the lone pairs of electrons. I've given a few hints in the paragraph after each problem to help you out. Feel free to check your answers at the end of the chapter AFTER you've given each one your best attempt.

<div>

```
              H           H

H      O      C      C      H

              H           H

   Ethanol
```

a)
</div>
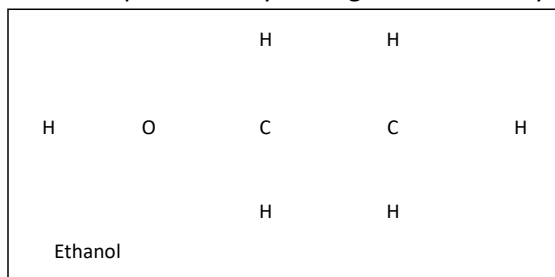
The best way to do problems like this, start off by drawing single bonds to connect all of the atoms.

Then, double check to make sure each atom has the number of bonds it normally has. If more bonds are needed for atoms to be "normal" then consider making double or triple bonds. In problem a, after all of the single bonds are drawn, every atom is "happy". The oxygen atom normally has two bonds and two lone pairs of electrons. To complete our structure, two sets of electron pairs need to be drawn on the oxygen atom.

<div>

```
   H                 H

       C       C

   H                 H

   Ethene
```

b)
</div>
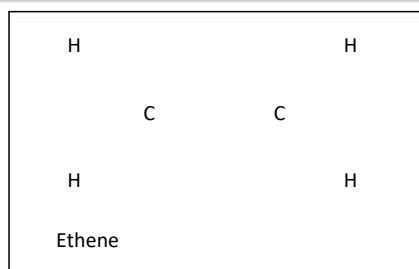
After drawing all of the single bonds in problem b, we notice that each carbon atom only has three bonds. Since each carbon atom wants four bonds, we need to make a double bond between the two carbon atoms.
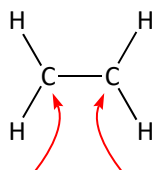
Not happy, has 3 bonds and wants 4. Need a double bond between these C's.

No electron pairs need to be drawn because each carbon atom usually has four bonds and no lone pairs of electrons.

c)

```
        H

H       C           C           N

        H

    Acetonitrile
```
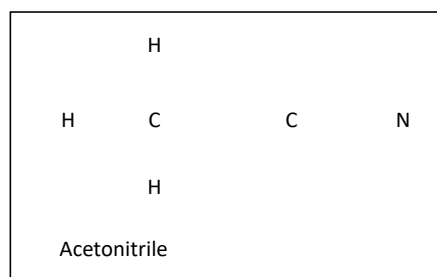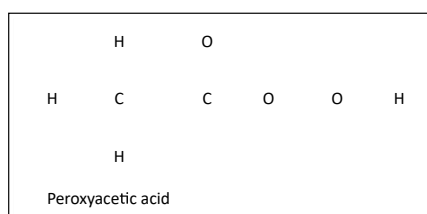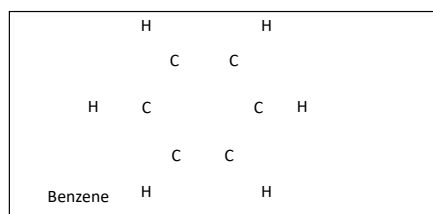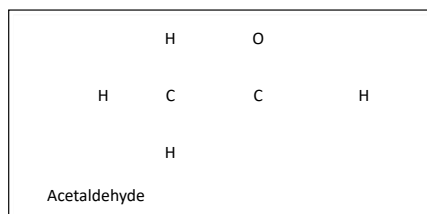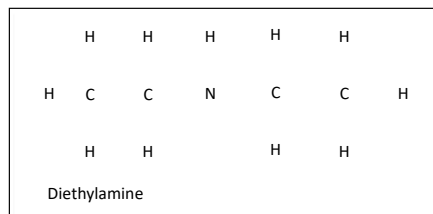
After drawing in all of the single bonds in problem c, we notice that the hydrogens and the first carbon are happy, but the second carbon atom and the nitrogen atom are not. We need to draw in more bonds, but make sure you don't draw a double bond between the two carbons, or that will make the first carbon have 5 bonds! That is a mortal sin to an organic chemistry professor! So, draw in a double bond between the second C and the N. They're still not happy. Can you see what we need to do to fix this problem?

d)
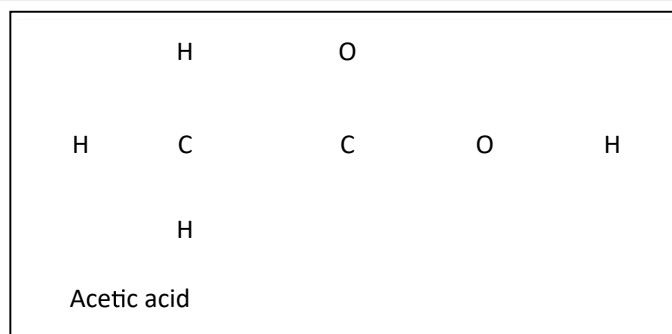
```
        H           O

H       C           C       O       H

        H

    Acetic acid
```

After drawing in all of the single bonds, we find that all of the atoms are happy except the second carbon and the top oxygen. This is a pretty easy fix by drawing in a double bond.

Try these next few problems on your own.

e)

```
    H   H   H   H   H

H   C   C   N   C   C   H

    H   H       H   H

    Diethylamine
```

```
            H       O

    H       C       C       H

            H

    Acetaldehyde
```

```
        H           H
            C   C

    H   C           C   H

            C   C

    Benzene  H          H
```

```
        H       O

    H   C       C   O   O   H

        H

    Peroxyacetic acid
```

2.6 Formal charges

An atom will have a negative charge if it contains an extra negative electron or two over what it normally has. An atom will have a positive charge if it contains one or two fewer negative electrons than it normally has. Chemists have agreed on a set of rules, or an accounting of electrons, to communicate how many electrons an atom has. This accounting is the atom's **formal charge**. Understanding formal charges will be useful to you later in this course. It is one way we can identify the reactive sites on molecules. It is crucial to understand formal charges in order to draw good resonance structures. Resonance structures will help you predict how a reaction will proceed.

2.5 Consider the following oxygen atom, :O: . This oxygen atom contains _____ negative electrons around it. Oxygen's placement in the periodic table tells us that it normally contains ____ negative electrons around it. Since this oxygen atom contains one more negative electron compared to normal, it has a -1 formal charge.

This oxygen atom, :O. . This oxygen atom contains _____ negative electrons around it. Normally, oxygen contains ____ negative electrons around it. Since this oxygen atom contains one fewer negative electron compared to normal, it has a +1 formal charge. That's pretty simple, right?

2.6 What are the formal charges of the following species? Two of the answers have been filled in for you as a self-check.

·O·   :O·   :O: :C·   ·C·   ·C·   :Cl: :N·   ·N·

+1 ___   ___   ___   ___   ___   ___   0 ___   ___
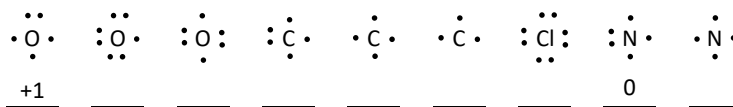
Usually, you will not be assigning formal charges to nonbonded atoms like the previous exercise. Instead, you will need to analyze atoms in molecules. When you analyze atoms in molecules, the trick is to remember which electrons are available to the atom. Every nonbonded electron is available to the atom. For every two electrons available in a bond, usually represented by a line (—), one-half of those electrons are available to be counted on the atom.
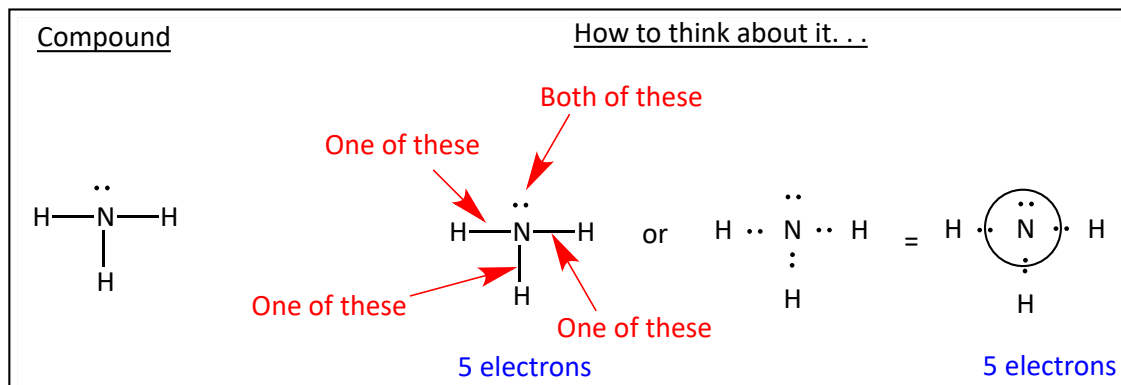
Let's look at the nitrogen atom in ammonia, NH_3.

Compound	How to think about it. . .

Both of these

One of these

One of these

One of these

H—N—H / H · · N · · H / or / = / H · N · H

5 electrons   5 electrons

Figure 2.22 Bonding of ammonia

Bonding and Structure

Normal nitrogen has five valence electrons. The nitrogen atom in ammonia has five valence electrons. Since it is normal, the nitrogen atom in ammonia has a zero formal charge. Zero formal charges are normally not written on atoms.

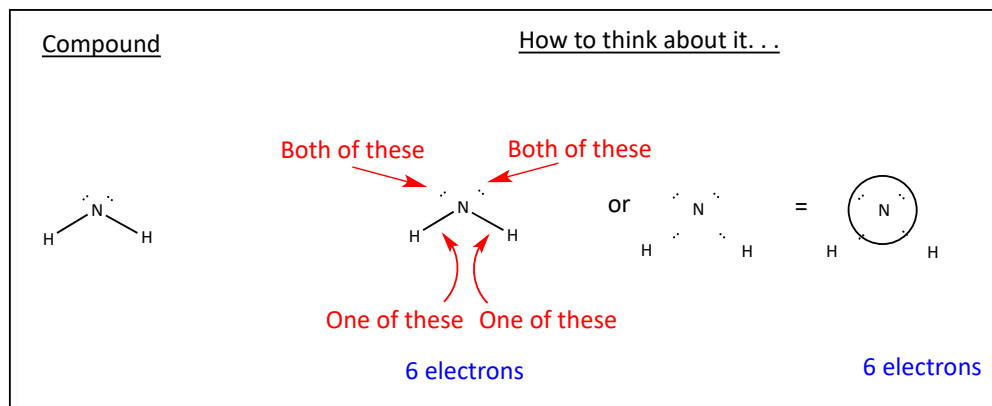The negatively charged amide ion (NH_2^-) has a nitrogen atom in a different electron environment.

Figure 2.23 Understanding formal charges in amide

Normal nitrogen has five valence electrons. The nitrogen atom in the amide anion has six valence electrons. Since it has one extra negative electron compared to what is normal, the nitrogen atom in amide has a -1 formal charge. Since this is a non-zero formal charge, it must be written on the nitrogen atom. If the formal charge is +1 or -1, typically the "1" is omitted and only the charge is written.
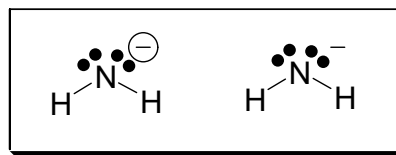
Let's analyze the nitrogen atom in the ammonium cation, NH_4^+.
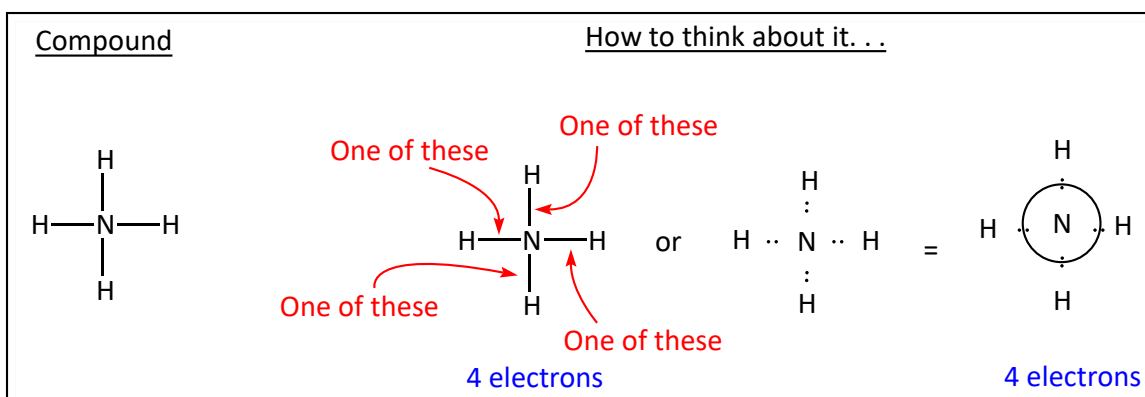
Figure 2.24 Understanding formal charges in the ammonium cation

Normal nitrogen has five valence electrons. The nitrogen atom in ammonium has four valence electrons. Since it has one fewer negative electron compared to what is normal, the nitrogen atom in ammonium has a +1 formal charge. Since this is a non-zero formal charge, it must be written on the nitrogen atom.
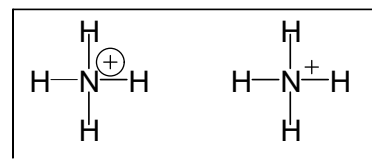
2.7 Identify the formal charges on the non-hydrogen atoms in the following structures. Write the formal charge on the atoms. If the formal charge is zero, do not write it.
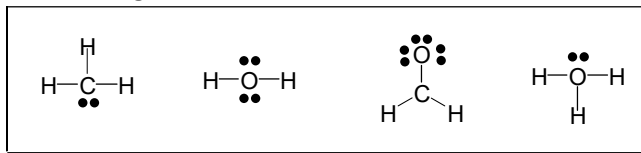
If you don't like to waste your time, it is important to be able to recognize when atoms are normal, with a zero formal charge, or not. Because if we have a molecule we are inspecting and it has dozens of atoms in it, we don't want to think about and analyze each of those atoms. This inspection of every atom would be a great waste of time. It is imperative that we be able to recognize normal bonding patterns. If we can quickly identify "normal" atoms, we can stop and analyze only the abnormal atoms. Take a moment to review the normal bonding patterns of atoms.

2.8 In the following molecules, try to quickly recognize the "normal" atoms with a zero formal charge, and then move on to the next atom. For the atoms that look abnormal, with a non-zero formal charge, stop and calculate its formal charge and write it on the atom.
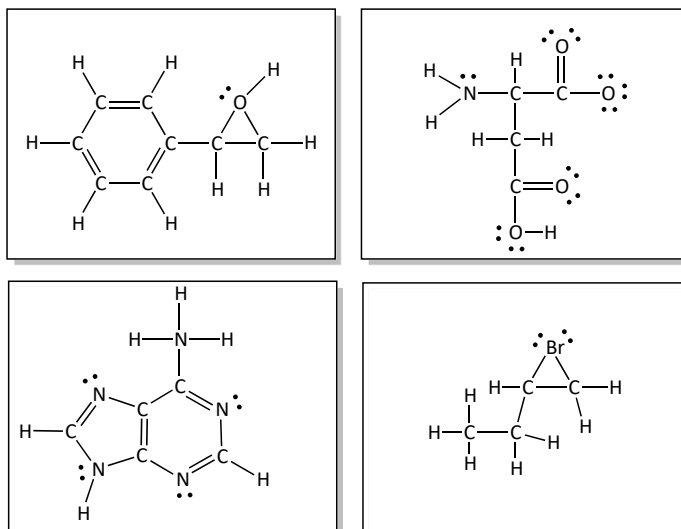
2.7 Drawing compounds

2.7.1 Condensed Structural Formula

Go back and review the normal, common bonding pattern for each atom. With these normal bonding patterns in mind, let's look at how organic compounds are typically drawn.

Let's consider the following alcohol. All atoms have a normal bonding pattern. Notice every carbon atom has four bonds, the oxygen atom has two bonds and two lone pairs and each hydrogen atom has one bond.
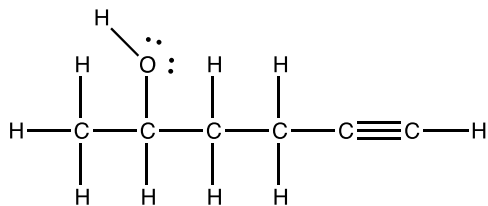
This drawing is perfectly acceptable. The problem with it is that it takes too long to draw in all of those hydrogen atoms. A quicker way to draw this compound is to not draw every bond to every hydrogen atom. A *condensed structural formula* is a drawing of a compound where the carbon-hydrogen bonds are not explicitly drawn. These may be drawn several ways.
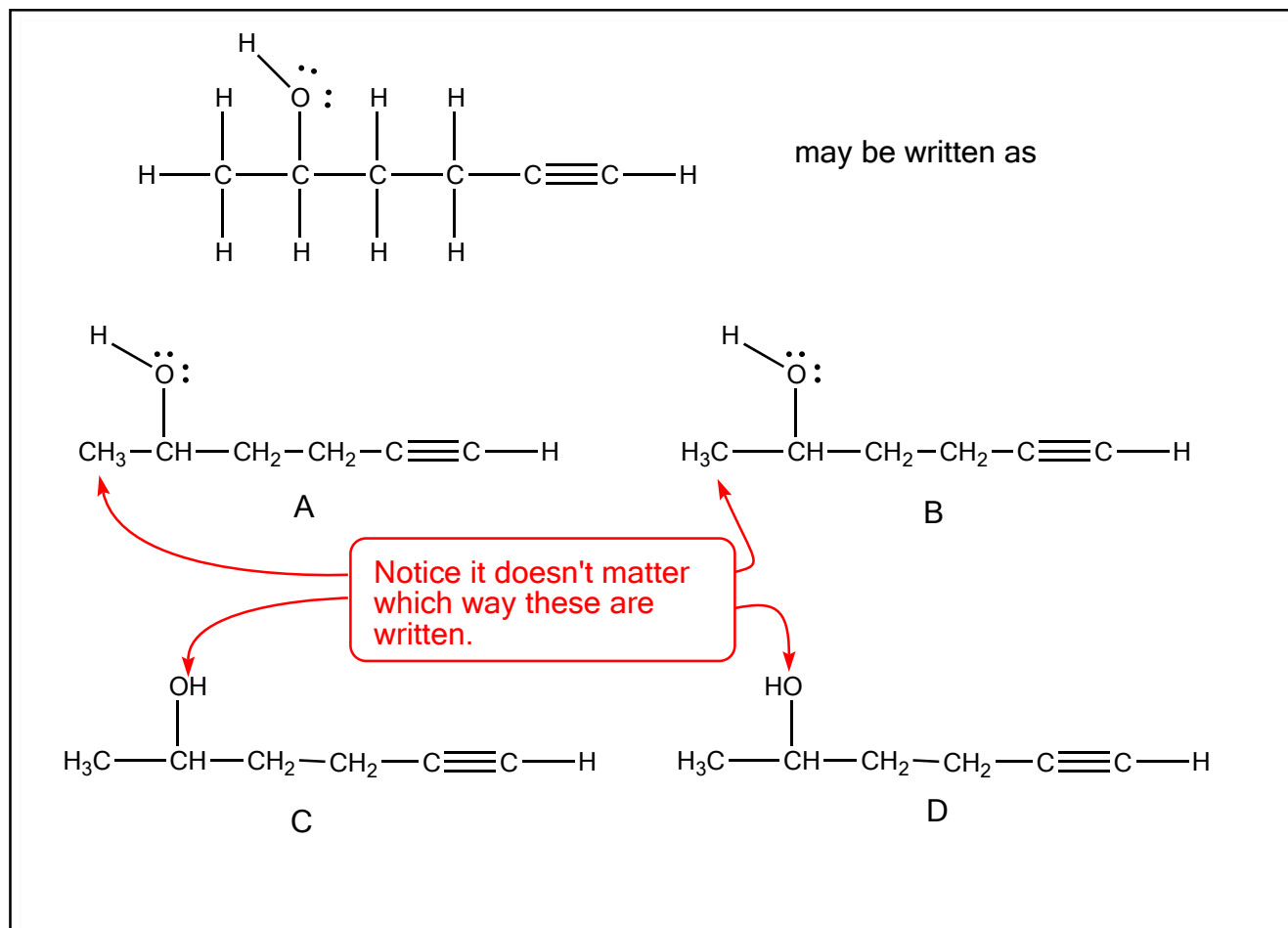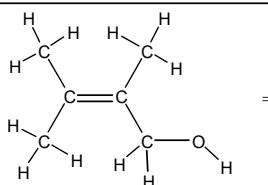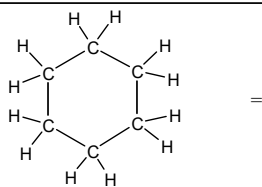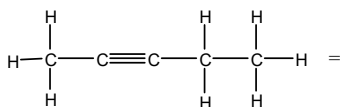

Figure 2.25 Drawing Condensed Structural Formulas

In compound A, all of the carbon-hydrogen bonds have been removed. The hydrogen atoms are usually written on the right of the carbon atom they are attached to. The exception to drawing the hydrogen atoms on the right of the carbon is shown in compound B. The carbon atom on the very left is drawn with the hydrogen atoms on the left. This may be done as it helps to show that the first and second carbon atoms are both bonded together. Compounds C and D show other ways to draw the OH. All of these are perfectly acceptable condensed structural formulas. I show them so you don't worry when you see subtle differences drawn.

2.9 Draw each of the following structures as a condensed structural formula.
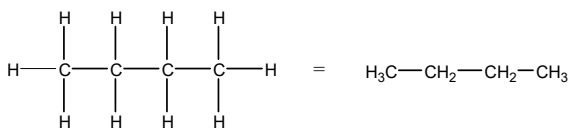
Instead of drawing out every bond, we can abbreviate the condensed structural formula if we have repeating groups. For instance, in the hexane, there are four methylene, CH_2, groups in the middle of the molecule. We can show this repeating group by putting it in parentheses and using a subscript to tell how many of them there are.

$$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3 = CH_3(CH_2)_4(CH_3)$$
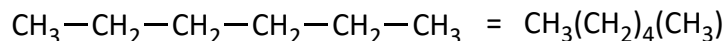
In this next molecule, there are two methyl, CH_3, groups on the same carbon atom. We can again use parentheses and a subscript to show this. There are three repeating methylene, CH_2, groups.

$$CH-CH_2-CH_2-CH_2-CH_3 = (CH_3)_2CH(CH_2)_3CH_3$$
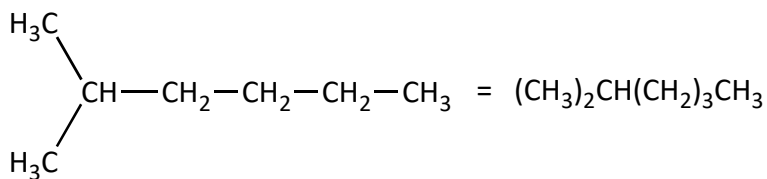
And, in this next molecule, there are three methyl groups, CH_3, on one carbon atom. There are four repeating methylene, CH_2, groups.

$$CH_3$$
$$H_3C—C—CH_2—CH_2—CH_2—CH_2—CH_3 = (CH_3)_3C(CH_2)_4CH_3$$
$$CH_3$$
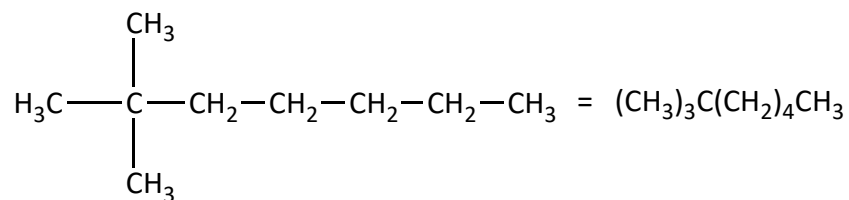
2.10 Draw the Lewis structure (every bond and atom) for the following molecules.

   a) $CH_3(CH_2)_3C(CH_3)_3$ b) $CH_3CH_2CH(CH_3)CH_2CH_3$ c) $C(CH_3)_4$ d) $CH_3(CH_2)_3CH_3$


2.7.2 Line Angle Formula

Chemists are smart, so they found a way to avoid drawing in all of those hydrogen atoms. If every practicing organic chemist knows that each carbon atom has four bonds, we could just not draw the H atoms at all. If we did not draw in the hydrogen atoms, and a chemist saw that the carbon atom only had two bonds drawn in, they would know that the carbon atom needs two more bonds to get to four, so it must have two hydrogen atoms attached. Remember, carbon atoms typically have four bonds. If you ever draw five bonds on a carbon atom, you might see your professor get angry. Trust me. You don't want to see your professor get angry. It is not pretty. It's funny what upsets an organic chemistry professor, isn't it?

Yikes!

Don't do this!
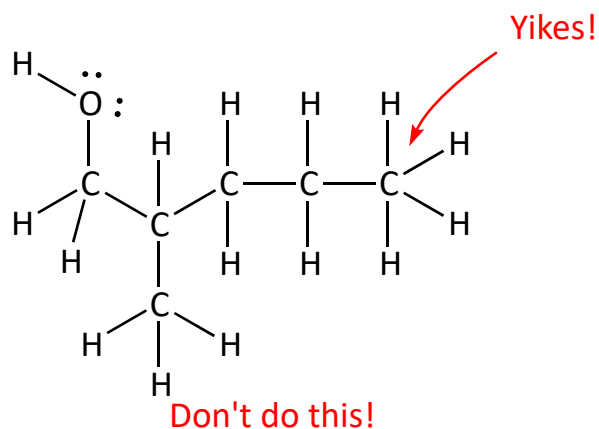
2.11 Draw in all of the missing hydrogen atoms on the following carbons.
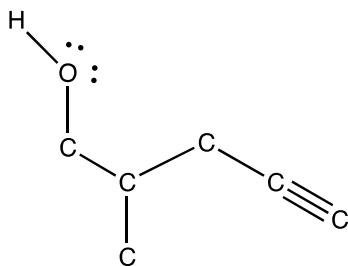
It's no fun drawing in all of those hydrogen atoms, is it? So, make sure you get good at drawing them using the other suggestions in this chapter! In fact, why draw in carbon atoms at all? Organic chemists have found an even easier-to-write notation. This notation is the line-angle formula or the line-angle structure. In the line-angle structure, a carbon atom is assumed every time a line ends, two lines come together at an angle, or a single bond meets a double or triple bond. So, instead of the above structure, chemists may write the following to save time.
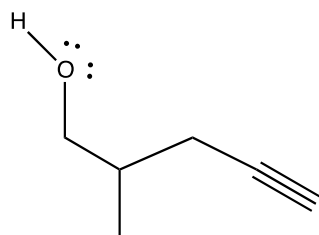
Notice that the hydrogen atom on the oxygen is still drawn in. It is customary to draw the hydrogen atoms that appear on all non-carbon atoms, also called *heteroatoms*. Let's make sure you can see where all of the carbon atoms are. Carbon atoms are located at the following sites.
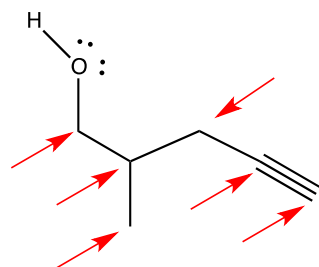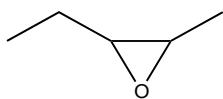
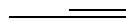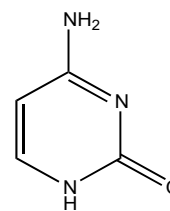2.12   Count the number of carbon atoms in the following compounds.
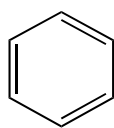
6
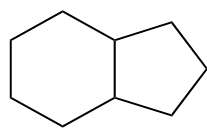
There is one more timesaving feature we can use to draw this compound. If practicing chemists know the normal bonding patterns, they can also figure out how many lone pairs of electrons are on atoms like nitrogen or oxygen. Normal oxygen has two bond and two lone pairs of electrons. So, our compound may be drawn like this.

2.13 Fill in the requested information.

How many hydrogen atoms are here? ____

How many lone pairs are here? ____

How many hydrogen atoms are here? ____

How many hydrogen atoms are here? ____
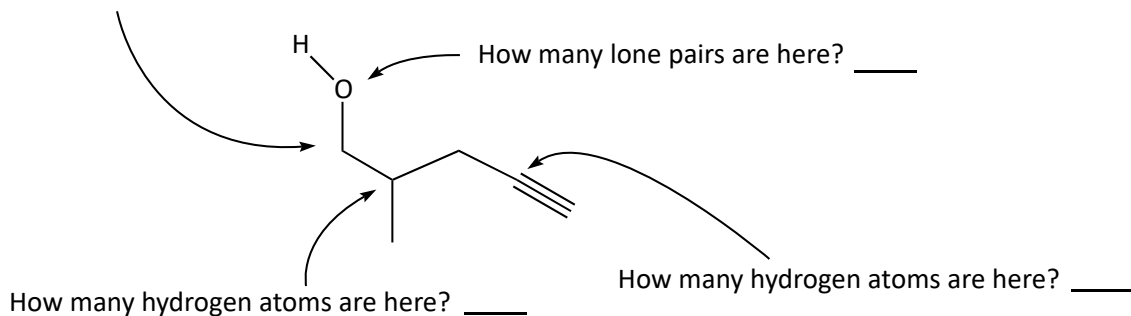
Most textbooks do not draw in the lone pairs of electrons. This is a rather unfortunate practice because many chemical reactions occur with these lone pairs. Oh well, we must remember to be diligent remembering how many lone pairs are on these heteroatoms. I like to draw them in so I do not forget they are there.
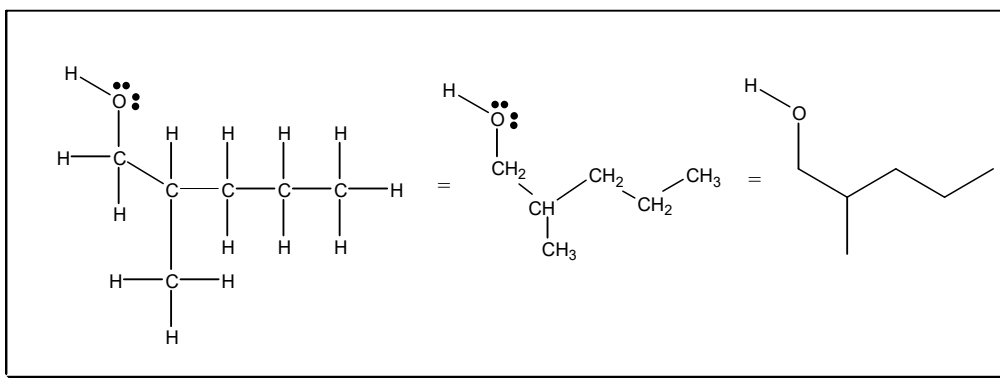
**2.14** How many lone pairs of electrons are on the following heteroatoms?

a)   b)   c) H_3C—C≡N d) H_3C—Br
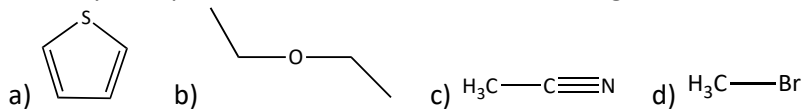
2.15 Identify the number of hydrogen atoms attached to each *carbon* atom.

a)   b)   c)   d) ═══   e)
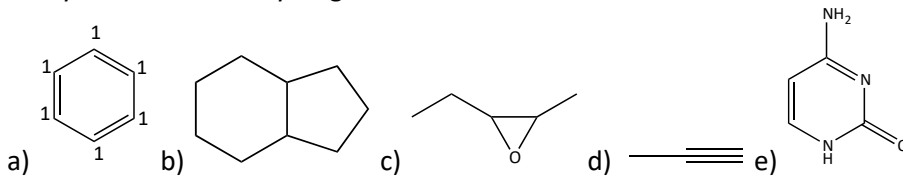
To review, these three structures are all equivalent.

There are a few other things you should know about drawing compounds. One is that single bonds on these compounds can rotate around. That means that the following drawings are all for the same compound. It does not matter which way you draw it.
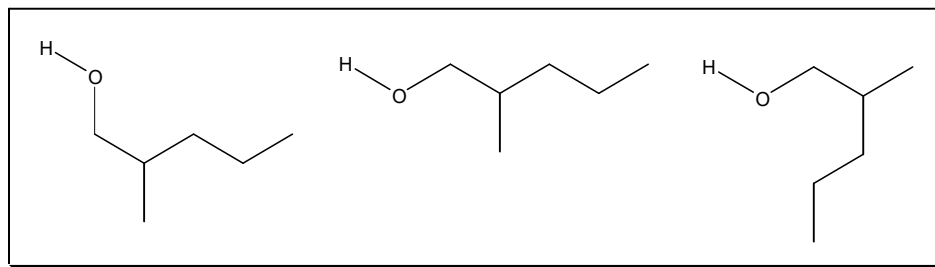
But, since the bonds all contain negative electrons, they repel each other. The bonds want to get as far away from each other as possible. Therefore, you would **not** want to draw this compound this way.

Yikes!
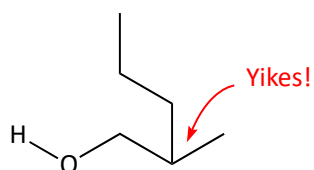
2.16   Draw the following compounds in the shorthand, line-angle notation.