CHAPTER

2

Representation of Organic Compounds

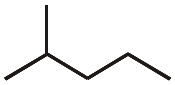
BOND-LINE DRAWINGS

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.

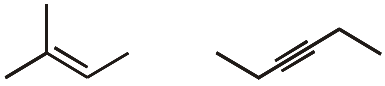
HOW TO READ BOND-LINE DRAWINGS

For example, the following compounds has 6 carbon atoms:

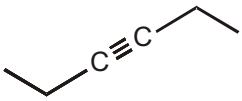
It is a common mistake to forget that the ends of lines represent carbon atoms as well. For example, the following molecule has six carbon atoms (Make sure you can count them)



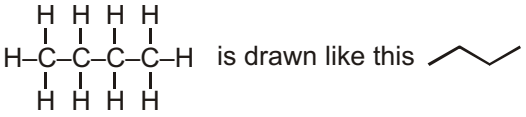
Double bonds are shown with two lines, and triple bonds are shown with three lines :

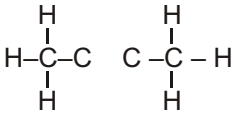


When drawings triple bonds, be sure to draw them in a straight line rather than zigzag, because triple bonds are linear (There will be more about this in the chapter on geometry). This can be quite confusing at first, because it can get hard to see just how many carbon atoms are in a triple bond, so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

 is the same as  so this compound has 6 carbon atoms

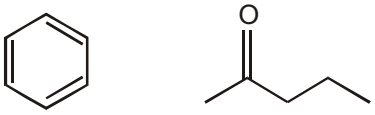
Don't let triple bonds confuse you. The two carbon atoms of the triple bond and the two carbons connected to them are drawn in a straight line. All other bonds are drawn as a zigzag:

 is drawn like this

But  is drawn like this 

Solved Example

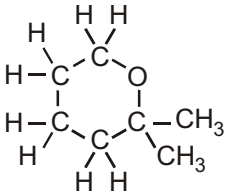
- Count the number of carbon atoms in each of the following drawings:



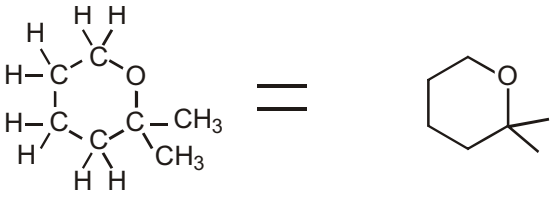
Ans. The first compound has six carbon atoms, and the second compound has five carbon atoms.

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:

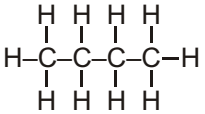


To draw this as a bond-line drawing, we focus on the carbon skeleton, making sure to draw any atoms other than C and H. All atoms other than carbon and hydrogen must be drawn. So the example above would look like this:

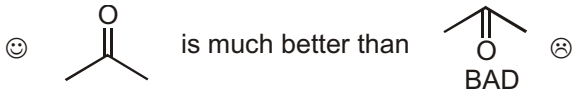


Points to Remember

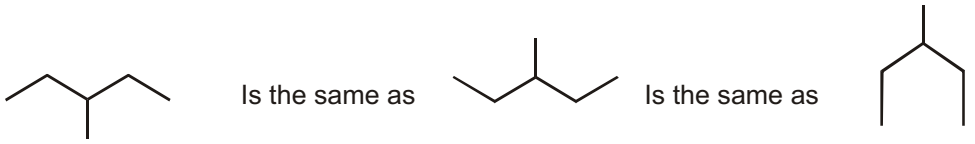
1. Don't forget that carbon atoms in a straight chain are drawn in a zigzag format:

 is drawn like this 

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

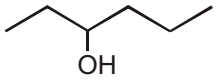
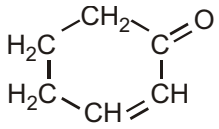
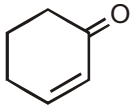
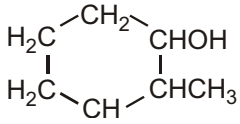
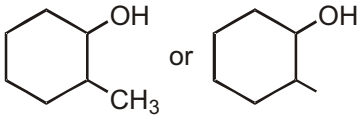
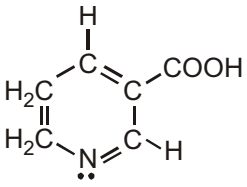
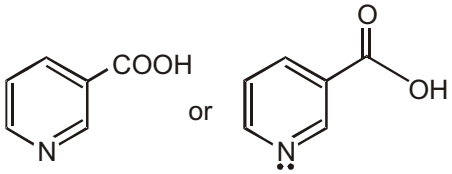


3. When drawing zigzags, it does not matter in which direction you start drawing:



LINE-ANGLE FORMULAS

Another kind of shorthand used for organic structures is the line-angle formula, sometimes called a skeletal structure or a stick figure. Line-angle formulas are often used for cyclic compounds and occasionally for noncyclic ones. In a stick figure, bonds are represented by lines, and carbon atoms are assumed to be present wherever two lines meet or a line begins or ends. Nitrogen, oxygen, and halogen atoms are shown, but hydrogen atoms are not usually drawn unless they are bonded to an atom that is drawn. Each carbon atom is assumed to have enough hydrogen atoms to give it a total of four bonds. Nonbonding electrons are rarely shown.\

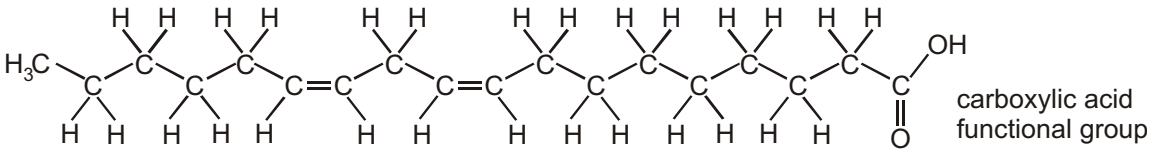
Compound	Condensed Structure	Line-angle Formula
hexane	$CH_3(CH_2)_4CH_3$	
hex-2-ene	$CH_3CH = CHCH_2CH_2CH_3$	
hexan-3-ol	$CH_3CH_2CH(OH)CH_2CH_2CH_3$	
cyclohex-2-en-1-one		
2-methylcyclohexan-1-ol		
nicotinic acid (a vitamin,also called niacin)		

❑ **NOTE:** IUPAC names will be discussed in next chapter.

DRAWING MOLECULES

Be realistic

Below is another organic structure—again, you may be familiar with the molecule it represents; it is a fatty acid commonly called linoleic acid.



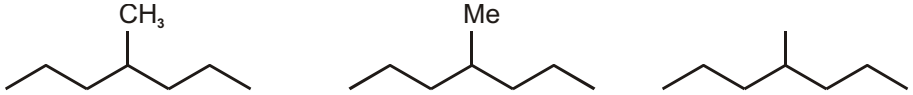
linoleic acid

We could also depict linoleic acid as

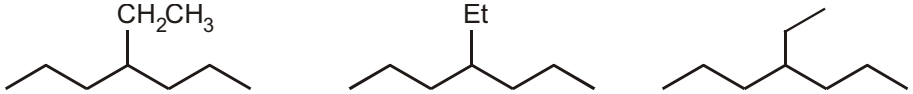
$CH_3CH_2CH_2CH_2CH\quad CHCH_2CH\quad CHCH_2CH_2CH_2CH_2CH_2CH_2CO_2H$

(Condensed formula)

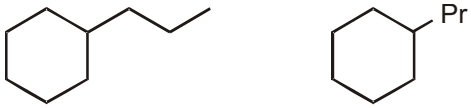
Methyl groups can be shown in a numbers of ways, and all of them are acceptable :



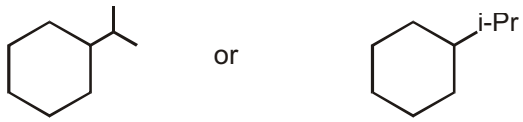
Ethyl groups can also be shown in a number of ways:



Propyl groups are usually just drawn, but sometimes you will see the term Pr (which stands for propyl):



Look at the propyl group above and you will notice that it is a small chain of 3 carbon atoms that is attached to the parent chain by the first carbon of the small chain. But what if it is attached by the middle carbon? Then it is not called propyl anymore :

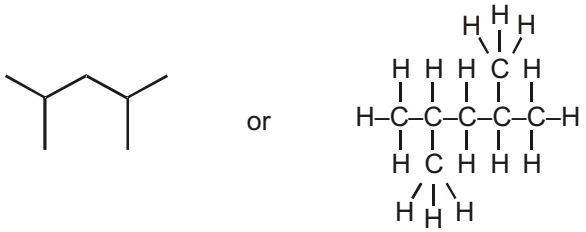


It is called as iso-Propyl or i-Pr.

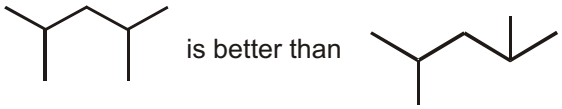
MISTAKES TO AVOID

Drawing where the C's and H's are not drawn. You cannot draw the C's without also drawing the H's:

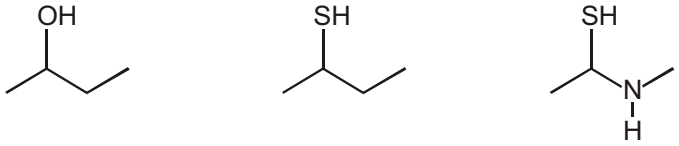
This drawing is no good. Either leave out the C's (which is preferable) or put in the H's:



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

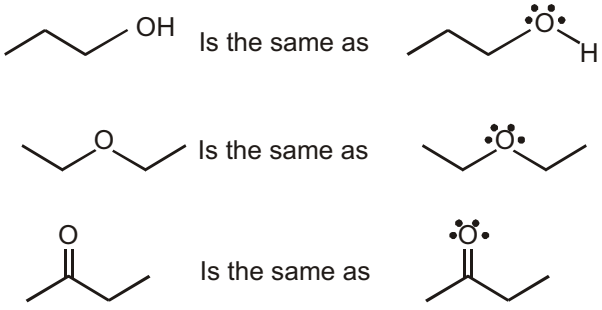


In bond-line drawings, we do draw any H's that are connected to atoms other than carbon. For example,

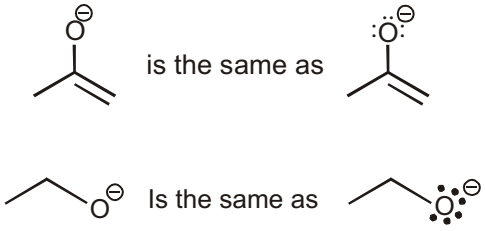


FINDING LONE PAIRS THAT ARE NOT DRAWN

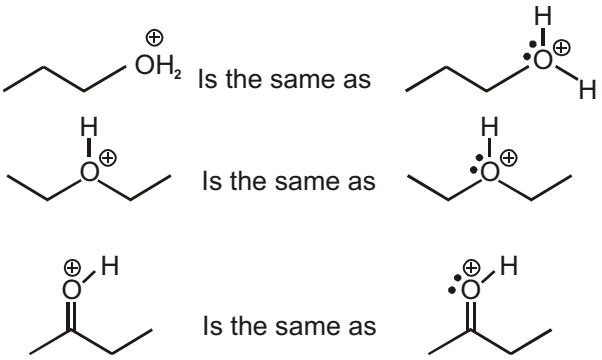
When oxygen has no formal charge, it will have two bonds and two lone pairs:



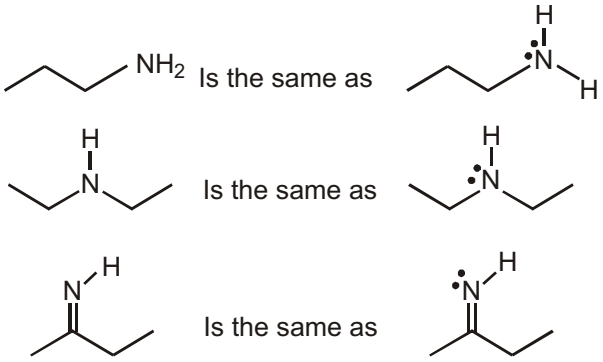
If oxygen has a negative formal charge, then it must have one bond and three lone pairs:



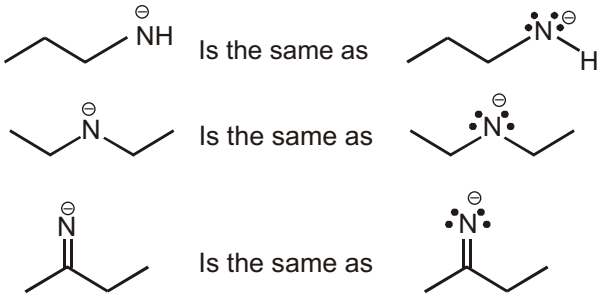
If oxygen has a positive charge, then it must have three bonds and one lone pair:



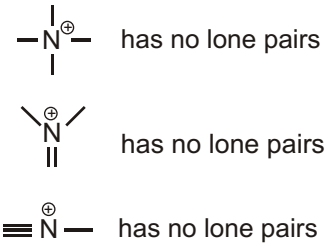
Now let's look at the common situations for nitrogen atoms. When nitrogen has no formal charge, it will have three bonds and one lone pair:



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

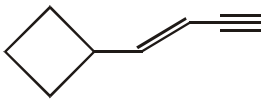


If nitrogen has a positive charge, then it must have four bonds and no lone pairs:



Solved Example

- The number of hydrogen atoms associated with the molecule shown below is ?

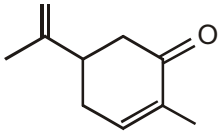


Ans. 10 hydrogens

INTERPRETING A BOND-LINE STRUCTURE

Solved Example

- Carvone, a substance responsible for the odor of spearmint, spearmint, has the following structure. Tell how many hydrogens are bonded to each carbon, and give the molecular formula of carvone.

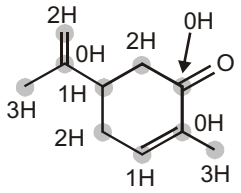


Carvone

Strategy

The end of a line represents a carbon atom with 3 hydrogens, CH_3; a two-way intersection is a carbon atom with 2 hydrogens, CH_2; a three-way intersection is a carbon atom with 1 hydrogen, CH; and a four-way intersection is a carbon atom with no attached hydrogens.

Sol.

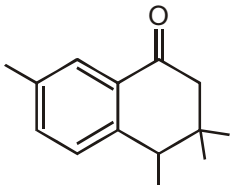


Carvone ($C_{10}H_{14}O$)

COUNTING THE NUMBER OF HYDROGEN ATOMS

Now that we know to count carbon atoms, we must learn how to count the hydrogen atoms in a bond-line drawing of a molecule. The hydrogen atoms are not shown, and this is why it is so easy and fast to draw bond-line drawings. Neutral carbon atoms always have a total of four bonds.

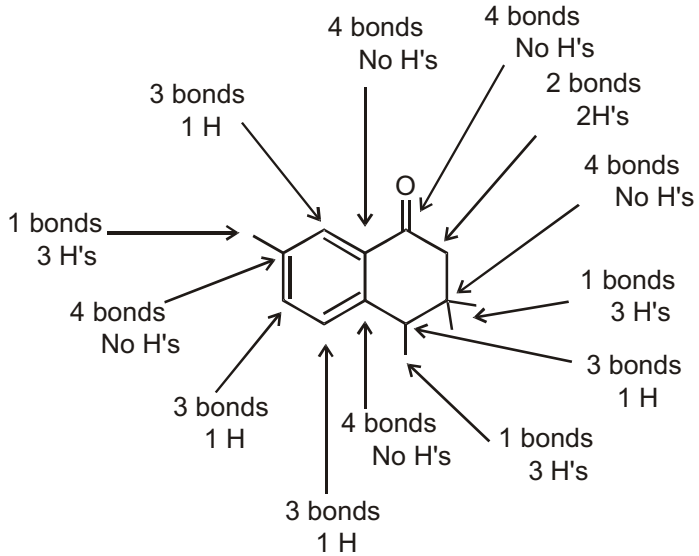
So you only need to count the number that you can see on a carbon atom, and then you know that there should be enough hydrogen atoms to give a total of four bonds to the carbon atom.



Solved Example

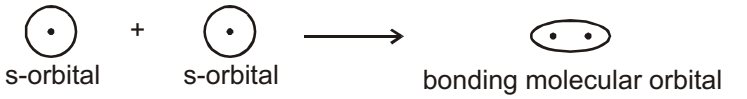
- The following molecule has 14 carbon atoms. Count the number of hydrogen atoms connected to each carbon atom

Ans.

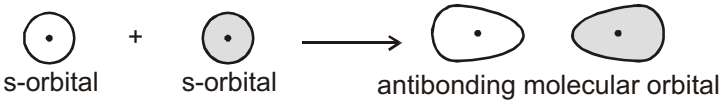


SIGMA (–) AND PI (–) BONDS

The electrons shared in a covalent bond result from overlap of atomic orbitals to give a new molecular orbital. Electrons in 1s and 2s orbitals combine to give sigma (–) bonds. When two 1s orbitals combine in phase, this produces a bonding molecular orbital.

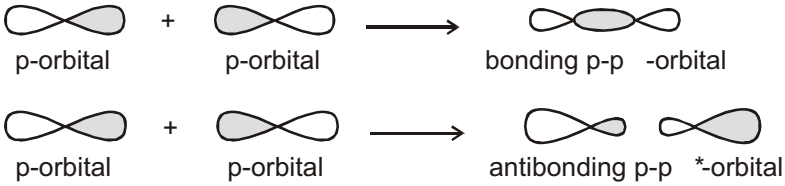


When two 1s orbitals combine out-of-phase, this produces an antibonding molecular orbital.

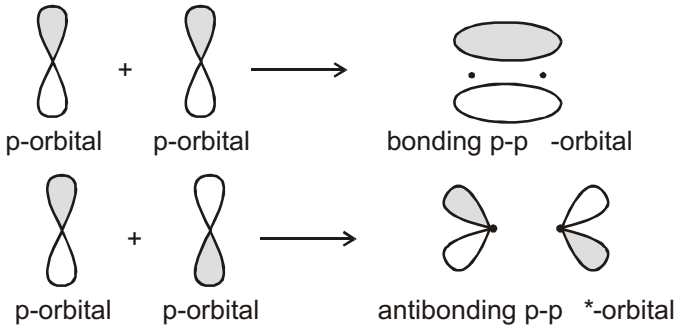


Electrons in p orbitals can combine to give sigma ( ) or pi ( ) bonds.

Sigma (-) bonds are strong bonds formed by head-on overlap of two atomic orbitals.



Pi(–) bonds are weaker bonds formed by side-on overlap of two -orbitals.

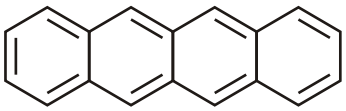


Only - or -bonds are present in organic compounds. All single bonds are s-bonds while all multiple (double or triple) bonds are composed of one s-bond and one or two p-bonds.

EXERCISE

SINGLE CHOICE QUESTIONS

1. Number of p-bonds present in given compound are:



(A) 8 (B) 9 (C) 10 (D) 12

2. How many Hydrogens does an alkane with 17 carbons have?

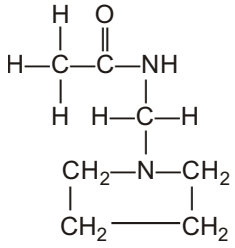
(A) 32 (B) 34 (C) 36 (D) 38

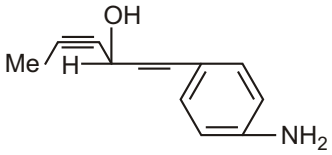
3. How many carbons does an alkane with 34 hydrogens have?

(A) 16 (B) 14 (C) 15 (D) 17

SUBJECTIVE TYPE QUESTIONS

1. What is wrong with these structures ? Suggest better ways of representing these molecules.



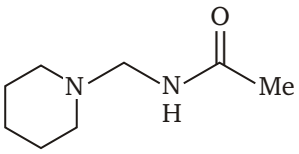


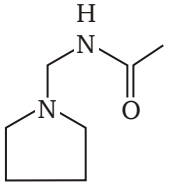
Purpose of the Problem

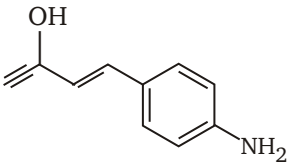
To shock you with two dreadful structure and to try and convince you that well drawn realistic structures are more attractive to the eye as well as easier to understand.

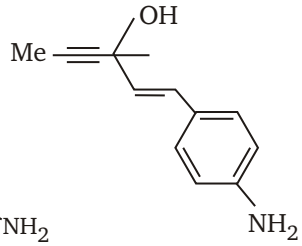
Suggested solution

The bond angles are grotesque with square planar saturated carbon, alkynes at 120°, alkenes at 180°, bonds coming off benzene rings at the wrong angle, and so on, The left-hand structure would be clear if most of the hydrogens were omitted. Hence there are two possible better structure for each molecule. There are many other correct possibilities.









Answers

Single Choice Questions

1. (B) **2.** (C) **3.** (A)

❑❑❑