BOAT AND CHAIR CONFORMATIONS

Cyclohexane, C_6H_{12}, is a ring of carbon atoms with two hydrogen atoms attached to each carbon atom. The skeletal formula for cyclohexane looks like a hexagon. A carbon atom is located at each vertex of the hexagon. Construct a model of cyclohexane by connecting 6 carbon atoms with sp^3 hybridization in a ring using the black bonds. Use the short (25mm) gray, links to add the 12 hydrogen atoms to the model of cyclohexane. The model of cyclohexane can be easily rotated between the "boat" and "chair" conformations.

Figure 8
"Boat" Conformation

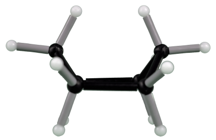
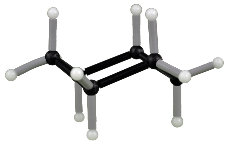


Figure 9
"Chair" Conformation



RESONANCE

When more than one Lewis structure can be drawn, the molecule or ion is said to have resonance. You can build the contributing structures of the acetate ion, Figure 10, or illustrate electron delocalization by spreading the pi bond across the region as shown in Figure 11. The two carbon-oxygen bonds are identical with a bond order (BO) of 1.5. In Figure 11 there is one sigma bond and half of a pi bond between each of the carbon and oxygen atoms and BO=1.5.

Figure 10: Contributing Structures

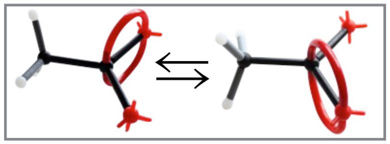


Figure 11: Electron Delocalization

AROMATICITY

The term aromaticity is used to describe a cyclic, planar molecule with a ring of resonance bonds. In benzene, there are six delocalized pi electrons over six carbon atoms essentially yielding half a pi bond together with the sigma bond for each pair of carbon atoms, giving a bond order of 1.5. Construct the model of benzene by using the black bonds to connect 6 carbon atoms having three sp^2 orbitals and one unhybridized p orbital. A closed loop of overlapping p orbitals must be present for aromaticity to occur. Using 12 connectors and 12 red, 40mm, links to represent the six pi electrons, build the 2 parts of the ring of delocalized electrons in benzene. Finally place the connectors onto the unybridized p orbitals of the carbon atoms as shown in Figure 12.

Figure 12: Aromaticity, Benzene

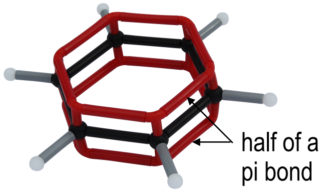


TABLE 1 THE ATOMS

Color	Atom	Symbol	Orbitals	Number
White	Hydrogen	H	1	28
Black	Carbon	C	4-sp^3 3-sp^2 and p 2-sp and two p	14 6 2
Red	Oxygen	O	4-sp^3 3-sp^2 and p 2-sp and two p	6 4 1
Blue	Nitrogen	N	4-sp^3 3-sp^2 and p 2-sp and two p	3 2 2
Green	Chlorine	Cl	1	6
Orange	Bromine	Br	1	2
Yellow	Fluorine	F	1	2
Purple	Iodine	I	1	2
Yellow	Sulfur	S	4-sp^3 3-sp^2 and p or sp^3d sp^3d^2	2 1 1
Purple	Phosphorus	P	4-sp^3 3-sp^2 and p or sp^3d	2 1

TABLE 2 THE BONDS

Color	Size	Use	Number
Gray	25mm	Use to link hydrogen atoms to the molecule	28
Black	40mm	Use to allow rotation around a single bond	18
Gray	50mm	Use to construct double and triple bonds	12
Red	83mm	Use to form pi bonds	6
Red	40mm	Each link represents 1/4 of a pi bond in a benzene ring	12
Red	—	Connectors for aromaticity	12

MEGA MOLECULES

ORGANIC CHEMISTRY PLUS

MOLECULAR MODEL SET

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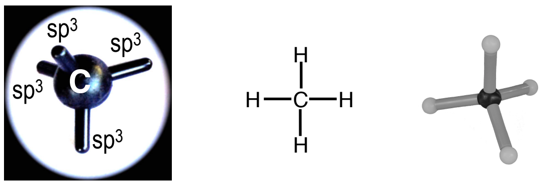
INTRODUCTION

The design of **MEGA MOLECULES** models is based on the hybridization of atomic orbitals and the valence bond theory. Hybridization is the concept of mixing atomic orbitals into new hybrid orbitals with new shapes and energies in order to form chemical bonds. Hybrid orbitals are very useful in the explanation of molecular geometry and atomic bonding properties. According to the valence bond theory, atoms join together by the overlap of atomic orbitals to form a molecule. In the model of methane, shown in Figure 1, a bond is formed by the overlap of an s orbital of hydrogen with an sp^3 hybrid orbital of carbon. The bond slides over the poles of the atom models and represents the region of orbital overlap. The models are manufactured to accurately represent the geometry of molecules as determined by crystallography. The bonds are scaled 1 inch (25mm) = 1 angstrom.

Figure 1: Model of Methane, CH_4



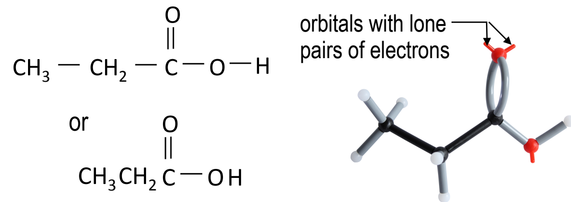
HOW TO BUILD A MOLECULAR MODEL

A molecular model can be constructed using a structural formula as your guide. A structural formula shows how the atoms of the molecule are joined together by various (single, double, or triple) chemical bonds and how the atoms and bonds are arranged in 3-dimensional space. There are four different types of structural formulas which show different levels of detail and types of information.

- Fully Displayed Formula (Expanded Formula)
- Semi-Displayed Formula (Condensed Formula)
- 3-Dimensional Formula (Dashed-Wedged Formula)
- Skeletal Formula (Bond-Line or Line-Angle Formula)

The fully displayed formula includes every atom and every bond. Compare the fully displayed formula for methane and the molecular model for methane shown in Figure 1. You need to remember that each line or bond represents a pair of shared electrons. In larger molecules, you can simplify the formula by writing CH_3 or CH_2 instead of showing all of the bonds. The semi-displayed formula for propanoic acid can be drawn as either of the formulas shown in Figure 2.

Figure 2: Semi-Displayed Formulas, Propanoic Acid

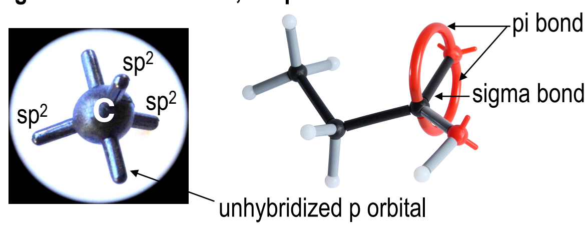


The double bond in propanoic acid can be constructed in two different ways.

<u>Method 1:</u> The carbon and oxygen models with four sp^3 orbitals are connected using two 50mm gray bonds as shown in Figure 2. Bend and slide the gray bonds over two of the poles on the atom models.

<u>Method 2:</u> Carbon and oxygen will hybridize to three sp^2 orbitals and one unhybridized p orbital when forming a double bond. Use atomic models of carbon and oxygen to construct the double bond as shown in Figure 3. Use a black bond to represent the sigma bond between the nuclei of the atoms. Illustrate the pi bond using 2 long (83mm) red bonds to connect the adjacent unhybridized p orbitals. This method allows you to clearly distinguish between sigma and pi bonds and shows the correct hybridization around the carbon atom.

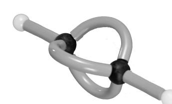
Figure 3: Double Bond, Propanoic Acid



Triple bonds (one sigma bond and two pi bonds) can also be constructed in two different ways.

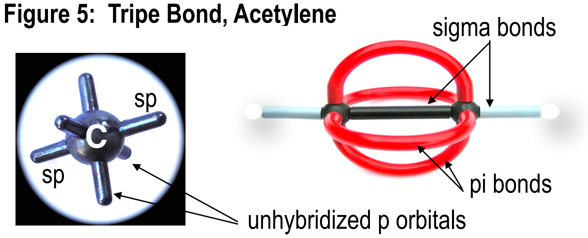
<u>Method 1:</u> Two carbon models with four sp^3 orbitals are connected using three 50mm gray bonds. This method illustrates the planarity of the molecule and the barrier to rotation that exists as a result of the pi bonds.

Figure 4: Triple Bond, Acetylene



<u>Method 2:</u> Carbon will hybridize to two sp orbitals and two unhybridized p orbitals when forming a triple bond. The molecule of acetylene, shown in Figure 5, has 2 pi bonds.

Figure 5: Tripe Bond, Acetylene



The purpose of the 3-dimensional formula is to provide more information than is given by a fully displayed formula by indicating approximate bond angles and orientations of bonds in space.

The symbols used are:

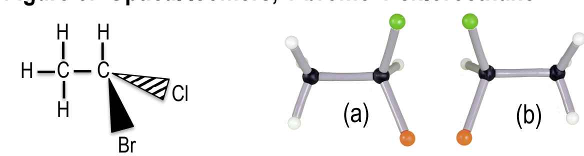
—— bonds that lie in the plane of the diagram

 bonds oriented towards the viewer

 bonds oriented away from the viewer

A common use for the 3-dimensional formula is to illustrate isomerism. The two models, shown in Figure 6, are not the same. They are optical isomers. Optical isomers are compounds which contain the same number and kinds of atoms and bonds, but different spatial arrangements of the atoms. Which model matches the 3-dimensional formula?

Figure 6: Optical Isomers, 1-bromo-1-chloroethane



The skeletal formula is the least detailed structural formula.

- There is a carbon atom at each junction between bonds in a chain and at the end of each bond.
- Enough hydrogen atoms are attached to each carbon atom to make each carbon atom have 4 bonds.
- Functional groups, such as –OH, an alcohol group, are shown in the skeletal formula.

Compare the skeletal formula for propanoic acid, Figure 7, with its semi-displayed formulas and model in Figure 2. There is a carbon atom at the beginning of the chain and at each junction between the bonds.

Figure 7: Skeletal Formula