USER GUIDE

for Molecular Model Set

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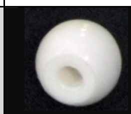
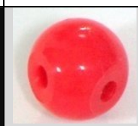
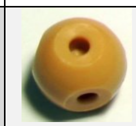
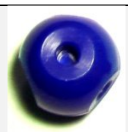
Models of organic molecules provide a physical representation of the three- dimensional arrangement of atoms in space. Using a molecular model kit for your study of organic chemistry will help you visualize molecular structures and relate the physical and chemical properties of the compound to its structure, as well as better understand both the chemical and physical properties of the molecules you encounter.

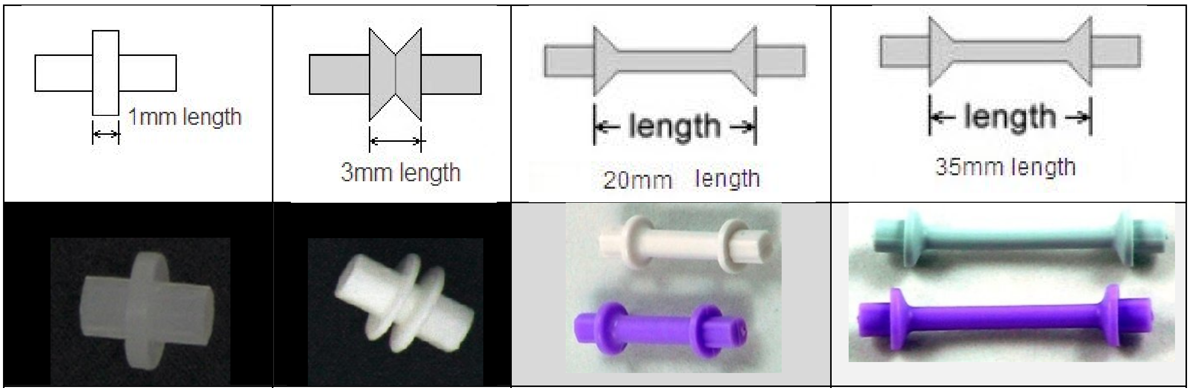
1 The first step to successfully using your molecular model kit is to become acquainted with the contents of your kit and what each unit represents.

   1.1 Your model kit contains several atoms and spheres that will represent the atoms you work with. The Atom Table below suggests the color for each atom and sphere. The hole on each atom represents the valence electrons.

Color	Black	White	Red	Blue	Yellow	Brown
						
Atom Represent	Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur	Phosphorus
	C	H	O	N	S	P

Color	Orange	Green	Dark Blue	Purple	Silver
					
Atom Represent	Fluorine	Chlorine	Bromine	Iodine	Metal
	F	Cl	Br	I	Metal

1.2 The Bond Table below specifies the *scaled* bond length represented by each of the connector in your kit along with a list of common bonds you will encounter throughout your study of organic chemistry and the corresponding connector that you should use.



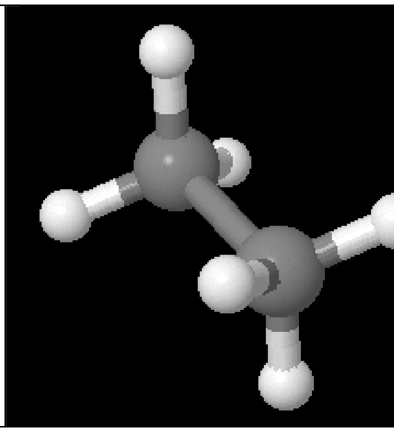
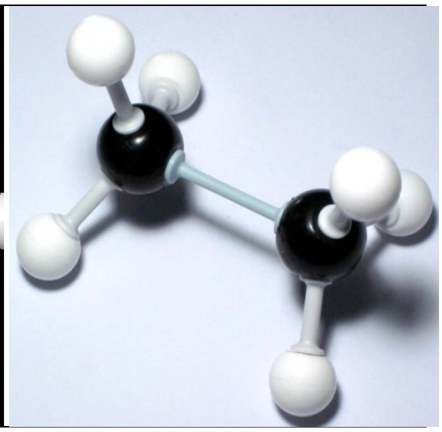
Single bond, space-filling, 1mm length, white color or transparent	Bond, 'V' shape, open model, 3mm length, white color	Single bond, open model, 20mm length, grey or purple color	Double or treble bond, open model, 35mm length, grey or purple color

2 Now that you are familiar with what your model kit contains, the next step is to learn how and when to use each unit.

2.1 When building a molecular model it will be helpful to designate which atom you will use for each atom in a molecular formula. Using different colors for different atoms will make it easier for you to keep track of atoms when creating and analyzing isomers. Furthermore, using the appropriate connectors to represent your bonds (single, double or triple) will enable you to better visualize which molecules can do resonance, which molecules are conjugated and/or aromatic, and which molecules have barrier(s) to rotation and are or are not planar. Keep in mind that while some bonds may be represented by more than one connector, it may be useful to pick connectors in a way that will make it easiest for you do recognize sigma and pi bonds.

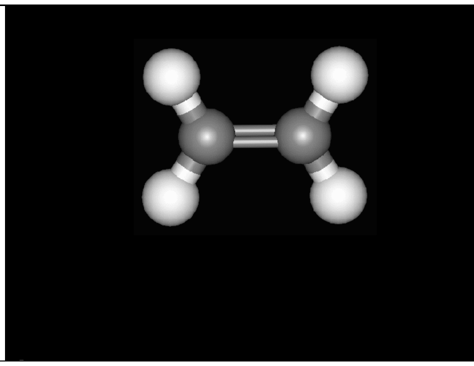
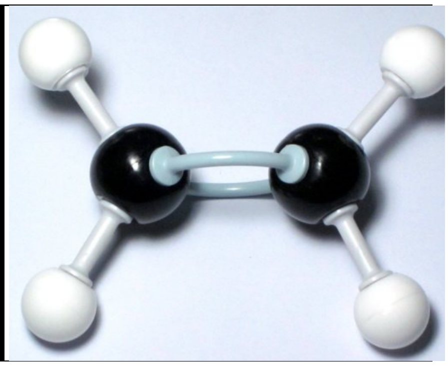
2.1.1 **Alkanes:** Single bonds are constructed by connecting two atoms or an atom and a sphere with a single connector (not including a blue connector) that corresponds to the atoms you are bonding.

Example : ethane (CH_3CH_3)

chemical formula: C_2H_6 structural formula: CH_3-CH_3		

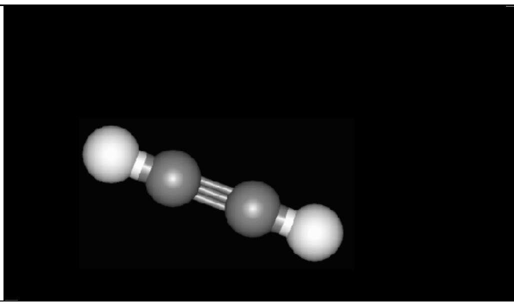
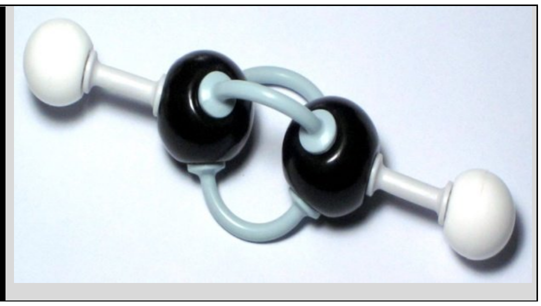
2.1.2 **Alkenes:** Two atoms (usually four-holed) are connected with two blue connectors. This method of construction highlights the planarity of a molecule and the barrier(s) to rotation that exist because of the pi bond.

Example : ethene (CH_2CH_2)

chemical formula: C_2H_4 structural formula: CH_2=CH_2		

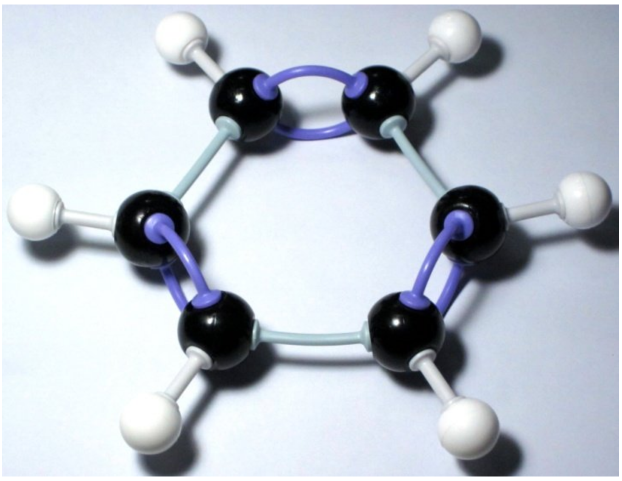
2.1.3 **Alkynes:** Two atoms (usually five-holed) are connected with three blue connectors. This method of construction highlights the barrier(s) to rotation that exist because of the two pi bonds.

Example : ethyne (HC≡CH)

chemical formula: C_2H_2 structural formula: CH≡CH		

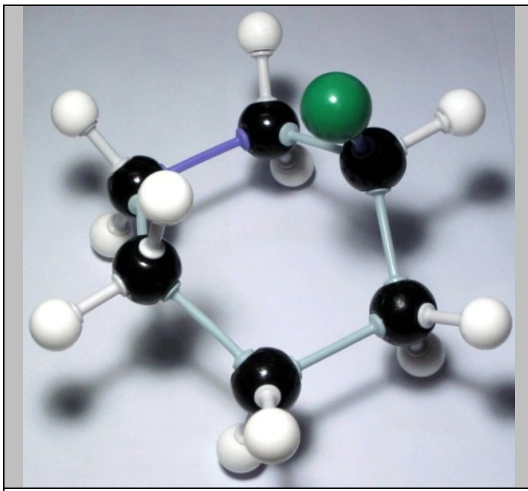
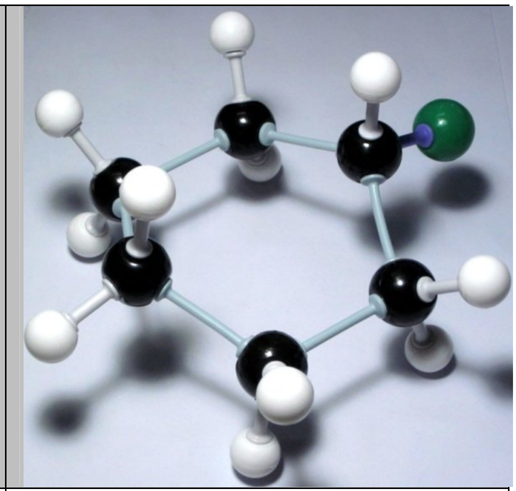
2.1.4 **Cyclic Molecules**: Cyclic alkanes, alkenes, and alkynes can be constructed using the same methods previously mentioned.

Example : Benzene (C_6H_6) is a common cyclic molecule (one that you will repeatedly encounter in your study of organic chemistry) that applies many of the model building rules listed above.



Furthermore, construction of cyclic molecules will enable you to better visualize chair conformations and *axial* and *equatorial* interactions for cyclic molecules with substituents. Mastery of this skill is critically important when dealing with carbohydrates.

Example : 1-chlorocyclohexane

	
(Cl = axial)	(Cl = equatorial)

* When building a molecular model, you will often encounter molecules that are not only composed of different atoms, but also of sets of the same atoms with different hybridizations.

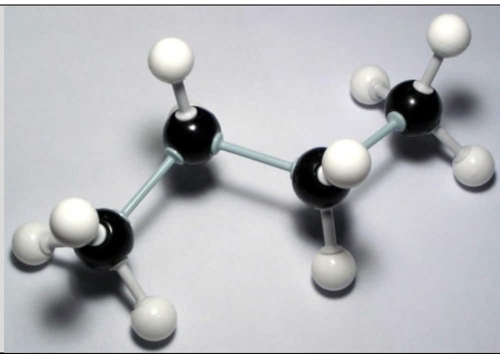
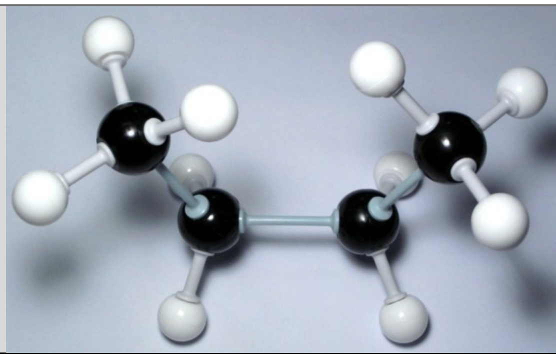
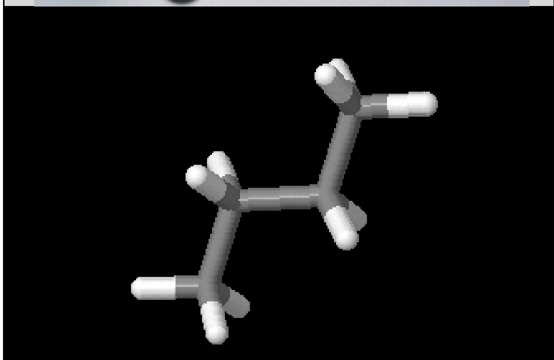
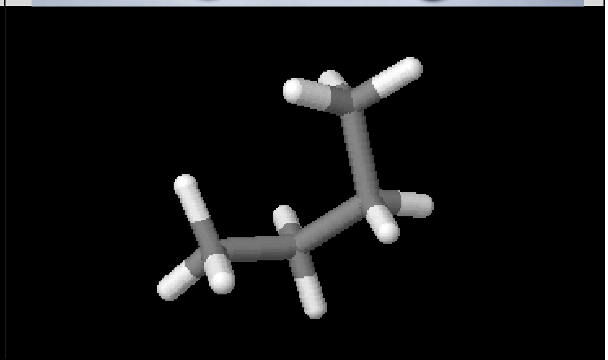
* C-H bonds do not always have to be used/included in your model in order for you to understand a molecules structure. However, if you are having a difficult time visualizing the formal charges [if any] or hybridization of the atoms in your molecule, it may be in your best interest to include them.

3 Now that you know how to use the contents of your model kit to construct various molecular structures, the next step is to learn how to use the structures you construct to help you better understand the characteristics of a molecule.

3.1 **Isomers** : Isomers are molecules with the same chemical formula but different spatial arrangements of atoms. Using the models you construct, you can alter the structure of your molecule to create different isomers.

3.1.1 **Conformational Isomers**: To create a conformational isomer you can rotate the substituent(s) of your molecule around a single bond. Rotating the substituent(s) of your molecule will enable you to visualize eclipsed and staggered (gauche and anti) conformations as well as determine whether your molecule is *sis* or *trans* . This in turn will enhance your understanding of the various types of strain and consequent relative energies of the isomers and conformations of the various molecules you will encounter throughout your study of organic chemistry.

Example : butane ($CH_3CH_2CH_2CH_3$)

	
	
anti butane	**bauche butane**

3.1.2 **Constitutional Isomers**: To create a constitutional isomer, you can alter the connectivity of the atoms that comprise your molecule to create different molecules. These molecules will have different structures and as a result will exhibit different properties.

3.1.3 **Stereoisomers**: There exist two types of stereoisomers (enantiomers and diastereomers). To create an enantiomer (nonsuperposable mirror image of a molecule) invert all of your molecules stereocenters by changing the position of one of the atoms around each stereocenter. To create a diastereomer invert at least one but not all of your molecules stereocenters by changing the position of one of the atoms around the stereocenter. The three-dimensional structure of your molecular models will also enable you to more easily determine the configurations of the stereocenter(s) of your molecule. To determine the configuration of the stereocenter(s) of your molecule, hold the atom or group of atoms with the lowest priority in your hand so that the stereocenter is facing you and so that the atom or group of atoms with the lowest priority is facing away from you. If the remaining atoms or groups of atoms facing you decrease clockwise in priority, the absolute configuration of your stereocenter is *R*. If the remaining atoms or groups of atoms facing you decrease counterclockwise in priority, the absolute configuration of your stereocenter is *S* .

3.2 **Resonance, Conjugation, & Aromaticity**: Building three-dimensional models of a molecules structure by using the various units in your model kit to depict not only the arrangement of atoms in space and their connectivity's but also the presence of *p* orbitals and lone pair electrons, will enable you to determine whether a molecule can do resonance, has conjugation, and/or is aromatic. This ability will greatly enhance your understanding of the properties of the molecules you encounter in organic chemistry.