

Molecular Structure Modeling Tutorial

Based on a Chemistry 14C extra credit project, fall 2008

(Note: all pictures were taken by me except the one that looks like Dr. H with his cat→).

The contents of the molecular structure model kit should provide some information about the types of atoms, bonds, or orbital plates that one should use to build molecular models. Certain atoms have specific numbers of holes specifically placed in certain locations so that it would correspond to approximately accurate bond angles in the molecules.



Atom

Parts code	Color	# of Holes	Bond Angle	Use
H	Pale blue	2	180°	Hydrogen
C ⁴	Black	4	109°	sp ³
C ⁵	Dark grey	5	90°	sp ² , dsp ³
O ⁴	Red	4	109°	sp ³
N ⁴	Dark blue	4	109°	sp ³
N ⁵	Light blue	5	90°, 120°	sp ² , dsp ³
Cl ⁴	Green	4	109°	sp ³
m ¹⁴	Light grey	14	90°, 109°, 125°	sp ³ , d ² sp ³

Bond

Bond #	Bond distance	Use
2	1.10 Å	C-H (pink)
4	1.40 Å	C=C (aqua)
6	1.54 Å	C-C (white)
7	1.80 Å	C-Cl (yellow)
10	1.33 Å	C=C (blue)

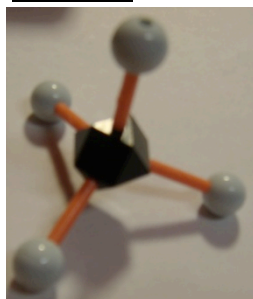
Orbital Plates

Item #	Use
BpG	P atomic orbital plate (green)
BpB	P atomic orbital plate (blue)

Introduction:

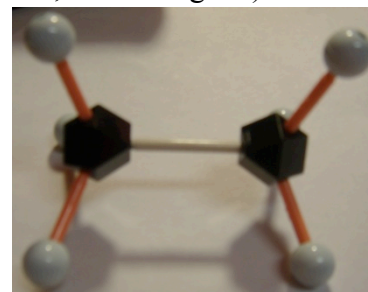
Models will provide 3D arrangement of the atoms which will help students visualize the correct orientation of the atoms and bonds in respect to each other. The molecular structure of a molecule gives information on molecular properties (i.e. physical, chemical, and biological).

Alkanes:



Methane: Use one black 4-hole polyhedron carbon and attach four light blue 2-hole spheres representing hydrogens using orange bond connectors for the C-H bond.

Ethane: Use one black 4-hole polyhedron carbon and attach it to another 4-hole polyhedron carbon

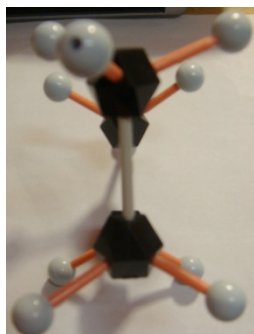


using white bond connectors for C-C single bond. Then attach six light blue hydrogens using orange bond connectors.

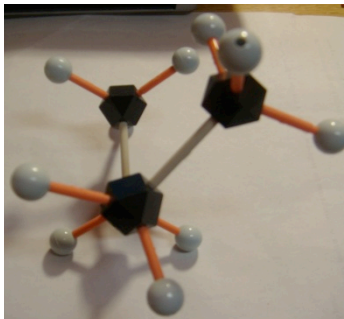
*****Test***:** Try making propane using three carbons, and 8 hydrogens.

Conformational Isomers: molecules with same structural formula (same connectivity) but different 3D conformations due to rotation about one or more σ bonds.

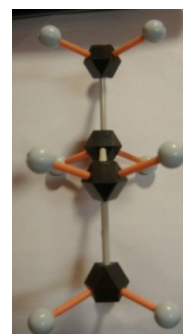
Rotation around a C-C single bond is relatively easy. Thus, there are an infinite number of conformational isomers (conformers). Butane ($\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$) can be rotated with ease around the C2-C3 bond to switch from its eclipsed conformations to staggered conformations of gauche and anti.



eclipsed



gauche



anti

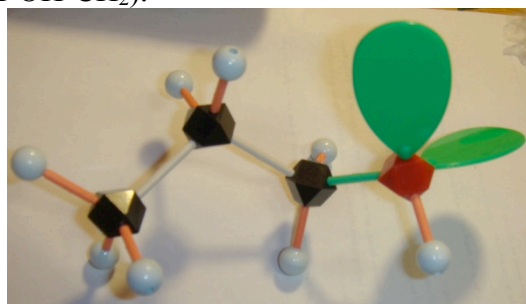
*****Test***:** Try making a cycloalkane with eclipsed, gauche, and anti conformations.

Alcohols (-OH)

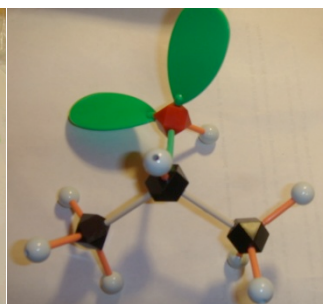
Remove one of the hydrogens and orange bond connector of alkane and replace it with one 4-hole red polyhedron using green bond, then add one hydrogen sphere with orange connector. You can add orbital plates in the other two holes for the lone pair electrons.

Structural Isomers: molecules with same molecular formula but different structural formula (different connectivity).

One can form 1-propanol ($\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$) by starting the model with the oxygen and then connecting the orbital plates, the hydrogen, and then the three carbon chain to the rest of the molecule. Or one can have the OH group attached to the 2nd carbon leading to (2-propanol) giving ($\text{CH}_3\text{CH-OH-CH}_2$).



1-propanol



2-propanol

*****Test***:** Try making a pentane, 1-pentanol, and 2-pentanol. See how many structural isomers you can make.

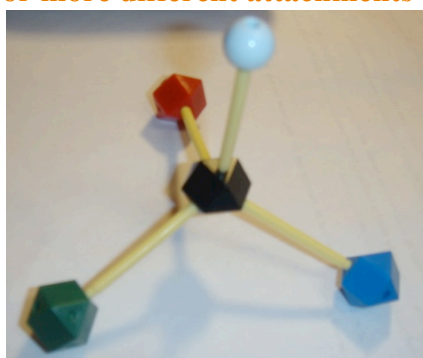
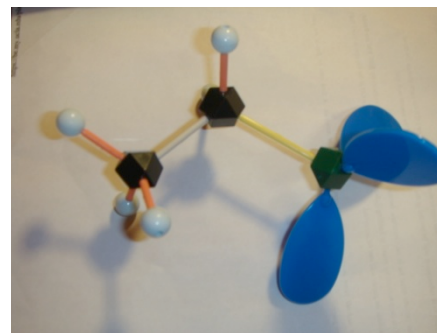
Haloalkanes-Alkyl Halides (C-X where X = F, Cl, Br, I)

Use the yellow connector for the C-X bond. The green four-hole polyhedron to represents any of the halogen atoms. Remember to add the three orbital plates to emphasize the halogen's three lone pairs.

*Bromoethane
(CH₃CH₂Br)*

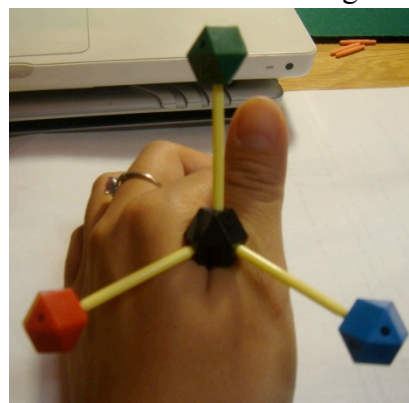
Stereoisomers: one of a set of isomers of same sequence of atomic attachments but differs in the position of the arrangements of atoms in space and cannot interconvert by rotation around a single bond.

Stereocenters: a carbon atom bearing four different attachments or an atom bearing three or more different attachments whose juxtaposition leads to stereoisomers.

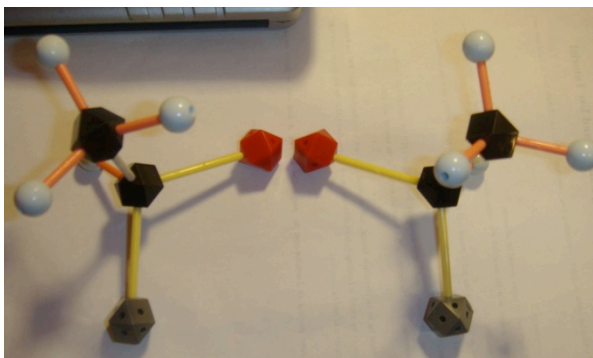


The stereocenter is sp^3 hybridized leading to two absolute configurations (R/S) that can be arranged for the specific stereocenter. The best way to look at a figure and determine R/S configurations is to make a simple molecule like the one below with a carbon center, a hydrogen attachment, an oxygen attachment, a halogen attachment, and a nitrogen attachment.. It does not really matter what the attachments are as long as you can tell them apart. Then, look at the stereocenter provided and number the priority groups from 1-4 depending on their atomic number. The largest

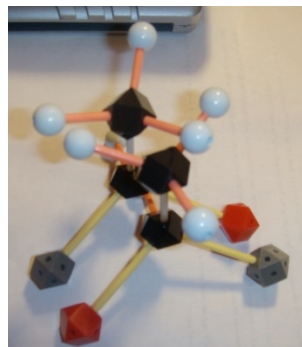
atomic number gets highest priority and the lowest atomic number (usually H gets the least). If one cannot deem priority by the bond connection, then look at the next atom out to determine the priorities. Now hold the hydrogen bond in the molecule that you just created and now you are looking at only three C-X, C-Y, and C-Z bond. Now look at your priority numbering from 1-3, if the order of 1 to 3 falls in a **clockwise** rotation then your molecular configuration is **R**. If it is in a **counterclockwise** rotation, then your molecular configuration is **S**. This takes some practice, so **practice!**



Construct model of 1-bromo-1-chloroethane (CH₃CHClBr) using 1 red polyhedron to represent chlorine and a gray polyhedron to represent bromine. (These colors were chosen so that the pictures are more clear, you can choose to make them both green polyhedrons since chlorine and bromine are both halogens.) Then make a second model in which two groups on carbon stereocenter are exchanged. These two models that you have just constructed are enantiomers.



R-1-bromo-1-chloroethane, S-1-bromo-1-chloroethane



nonsuperimposable

Enantiomers: one of a pair of stereoisomers that are nonsuperimposable mirror images.

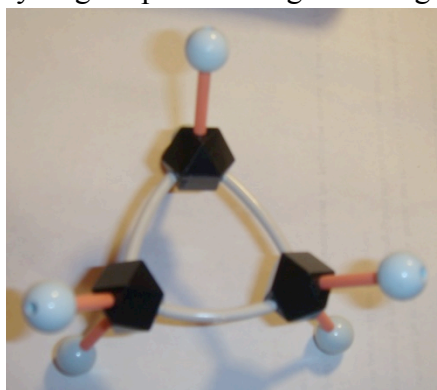
Diastereomers: stereoisomers that is not an enantiomer

Meso compounds: an achiral compound that contains two or more stereocenters.

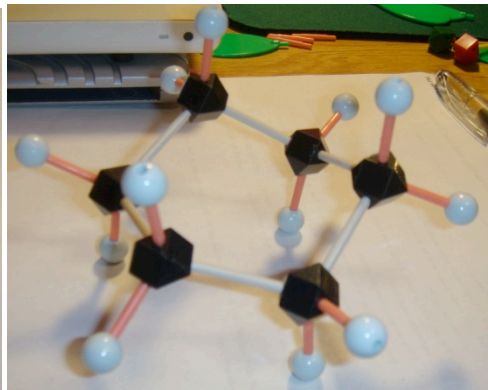
*****Test***:** Practice making 1-bromo-1-chloroethane in both the R and S configurations.

Cycloalkanes

Use the 4-hole black polyhedron for carbon atoms, white connector of C-C bonds. Then connect the hydrogen spheres using the orange connectors.



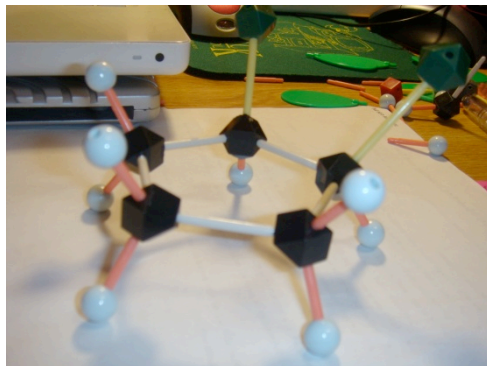
cyclopropane



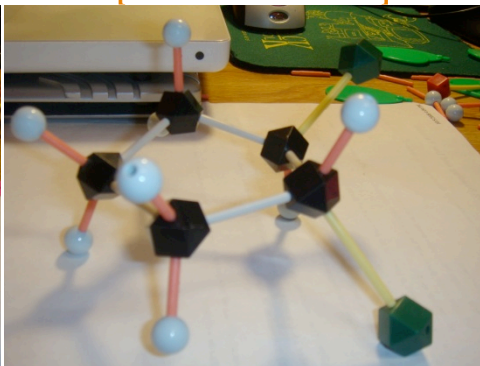
cyclohexane

*****Test***:** Practice making cyclooctane (8 carbons). What shape is it in? (hint: it is something that is in a restroom and can hold lots of water)

Cis/Trans Isomers: when two substituents are attached to the ring on different carbons, then it can be either in the cis or trans conformations. [cis = zee zame zide]

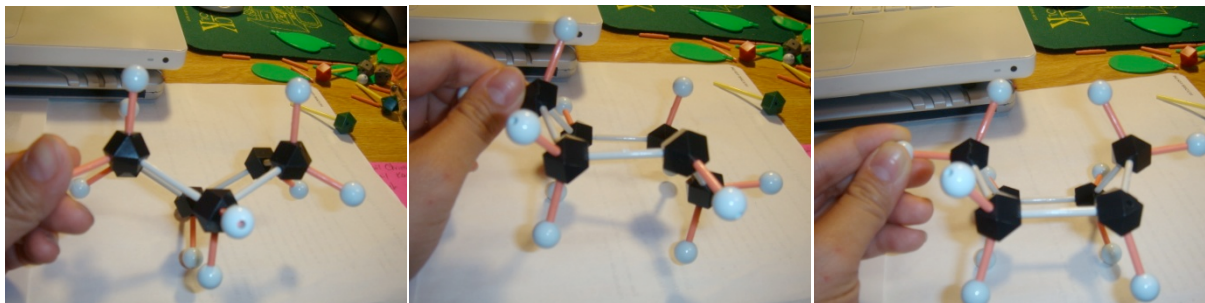


cis



trans

Cyclohexane (C₆H₁₂) is an important molecule because of its unique biological, chemical and conformational properties. Thus, it is a favorite on EXAMS!!! The chair conformation can be made if you hold carbons 2, 3, 5, and 6 in plane while pushing carbons 1, 4 below plane. The ring-flip can be done by pushing carbon 1 down and carbon 4 up while holding carbons 2, 3, 4, and 6 still. The boat conformation can be created by pushing carbons 1 and 4 to the same side while hold the rest of molecule stable.



chair

ring-flip

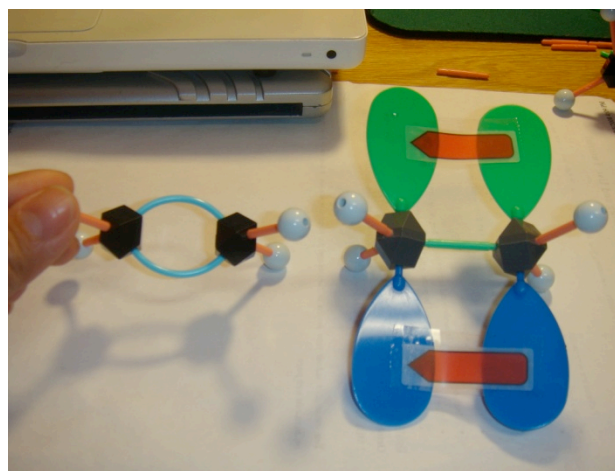
boat

*****Test***:** Practice making the cyclohexane chair, ring-flip and boat conformations. It is for your own good, I promise!

Alkenes:

Carbon atom in a double bond is sp² hybridized and is attached to only two other groups. There are several ways of depicting a C=C bond. We will be making ethene (C₂H₄)

- 1) Join two 4-hole black polyhedron carbon atoms with two blue curved connectors that are slightly curved. All atoms in figure are in the same plane emphasizing the planarity of the system and the barrier to rotation caused by the double bond.



- 2) Connect two 5-hole grey polyhedral with green connector at the small square rectangular faces to represent sp²-sp² sigma bond. The other coplanar holes allow for attachment of the rest of substituents. Then insert two orbital plates in each of the triangular faces of the carbon atoms to represent the p-orbital. This model shows the double bond as a sigma (green connector) as well as a pi bond (orbital plates). Connect orbitals with tape if you want to show the rigidity of the pi bond.

*****Aldehydes & Ketones & Imines** are compounds with double bonds between C=O or C=N.

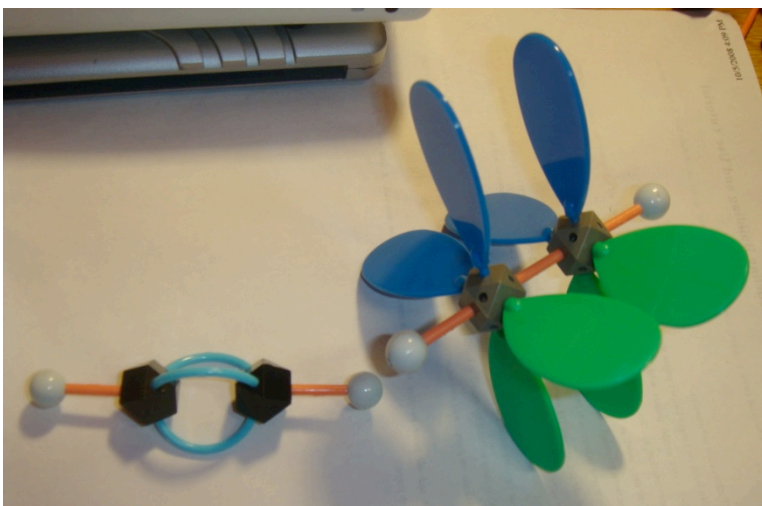
Alkynes:

Carbon atom in a triple bond is sp hybridized and is attached to only one other substituent. There are two methods of constructing a triple bond as well. We will be making ethyne (C₂H₂)

- 1) Use three blue curved connectors to connect three of the holes in 2 of the 4-hole black polyhedron carbon. Insert the other group to remaining hole.

- 2) Other method is to depict the triple bond as a sigma bond and two pi bonds. Use an orange connector to join the two gray 14-hole carbon. Attach a light blue sphere to each gray polyhedron with orange connector. Insert two orbital plates of each color in four remaining holes placing different colors opposite of each other. Make sure that the orbitals line up to represent the barrier to rotation as well as planarity of a triple bond.

*****Nitriles** are compounds with triple bonds between $C\equiv N$ so you can depict them using the same method as described above to represent the sigma bond by the plastic connector and the two pi bonds by the orbital plates.



Benzenes

Benzenes (C_6H_6) are aromatic, conjugated, and have resonance structures. Thus, they are very stable molecules. They are also very important and appear a lot in exams!!!

*****Test*****: What are the two methods for making benzenes? Are they the same as the alkene methods? Why? (Answer: BELOW)

- 1) Use six 4-hole black polyhedron for carbon atoms. Connect each black piece to another with two blue connectors and to the second carbon with white connector bond. Then attach one light blue sphere to each carbon with an orange connector. (Benzene does not necessarily have alternating single-double-single bond, but rather a resonance somewhere between the single and double bond.) The model is correct, however, in the fact that the molecule is planar and it has a barrier to rotation due to the cyclic, aromatic structure as well as the partial pi bonds in each of the C-C bonds.
- 2) Use six 5-hole grey polyhedron and connect them at the rectangular phases using the green bonds. Make sure that all the carbons line up in a plane. Then add one hydrogen to the other side of the rectangular face, one for each carbon atom. Now add the orbital plates to the triangular faces of the carbon atoms, using the green orbital plates on the top and the blue orbital plates on the bottom making sure that all orbitals line up. The orbital plates represent the electron cloud of the aromatic benzene molecule.

