

MOLECULAR STRUCTURE

For each of the following molecules, make the models and then draw the models. Until the last page, use tetravalent atoms. Make double bonds by using two of the soft, flexible white bonds to make “banana double bonds”.

- For molecules involving lone-pairs, draw them with the lone pairs shown.

Guidelines for Drawing Models:

A. 3-D Perspective

1. Keep as many atoms as possible in a single plane (plane of the paper) by zig-zagging. Connections within the paper are drawn with straight lines.
2. Use wedges to indicate atoms that are in front of the plane.
3. Use hashes to indicate atoms behind the plane.

B. For any tetrahedral atom, only 2 attachments can be in the plane, 1 must be in front, and 1 behind.

-if the two in the plane are “down”, the hash/wedge should be up

-if the two in plane are “up”, the hash/wedge should be down.

-the hash/wedge should never point in same direction as the in-plane lines, or else the atom doesn't look tetrahedral

-for polyatomic molecules, it is strongly preferable to NOT have either of the in-plane atoms pointing straight up. Straight-up in-plane atoms do not lend themselves to extended 3-D structures.



Good! Look tetrahedral



Bad! These don't look tetrahedral!

1. ALKANE. butane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$

-take the chain and wiggle around all the single bonds.

-The most stable actual shape is the one with the carbons zig-zagged and co-planar.

-Notice the symmetry possible.

2. ALKANE. Pentane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$

3. HALOALKANE. 2-bromobutane, $\text{CH}_3\text{CHBrCH}_2\text{CH}_3$

-notice that if the 4 carbons are co-planar zig-zagged, the attached Br can't be in the same plane.

-try to compare with a partner 2 cases in which Br is in front versus behind. Are they the same molecule, or isomers?

4. ALKENE. Draw both: a) trans-2-butene, $\text{CH}_3\text{CH}=\text{CHCH}_3$
and b) cis-2-butene

(trans means the two CH_3 groups are on the opposite sides of the double bond; cis means they are on same side)

-notice that not only the 2 double-bonded C's but also the four atoms directly attached are all co-planar.

5. ALKYNE. 2-butyne, CH_3CCCH_3

-draw Lewis structure first

6. WATER. H_2O

-DRAW at least 4 different orientations, and specify the lone-pairs.

-try to have at least one picture in which all of the atoms are in the plane of the paper.

-For building the model, visualize a lone-pair by using a stick without an atom at the end.

-draw in the lone pairs for this and all following pictures. (For this assignment; not normally required for class!)

7. ALCOHOL. Ethanol, $\text{CH}_3\text{CH}_2\text{OH}$

8. ETHER. Diethyl ether, $\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$

9. FORMALDEHYDE. CH_2O .

-for 9-16, make sure you draw the Lewis structure before you build models and draw the 3-D picture. If you don't know the connectivity, you have no chance!

10. ALDEHYDE. $\text{CH}_3\text{CH}_2\text{CHO}$.

11. KETONE. $\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_3$.

12. ACID. $\text{CH}_3\text{CH}_2\text{CO}_2\text{H}$.

13. ESTER. $\text{CH}_3\text{CH}_2\text{CO}_2\text{CH}_3$.

14. AMMONIA. NH_3

15. AMINE. $(\text{CH}_3\text{CH}_2)_2\text{NH}$

16. AMIDE CH_3CONH_2 .

17. CYCLIC COMPOUNDS A. Cyclopropane (CH₂)₃

-notice how hard this is, how the bonds “bend”, etc.. Real cyclopropane experiences real “ring strain” based on the impossibility of achieving 109° bond angles.

18. Things that can't be completely drawn “3-D”. 2-methylbutane, CH₃CH₂CH(CH₃)₂
-notice that not all 5 of the carbons can be coplanar. Structures like this can't be illustrated completely or easily. What you should do is simply draw “CH₃” as being out-of-plane, but don't try to illustrate the “3-D-ness” of that carbon. Ask instructor for confirmation.

19. CYCLIC COMPOUNDS B. Cyclohexane (CH₂)₆

-Don't bother to draw! Too tough! But do build the model.

1) notice that the 6 carbons do not easily remain coplanar. By puckering, ideal 109° bond angles can be achieved.

2) In the best model, 3 H's point straight down, 3 H's point straight up, and 6 H's essentially extend almost horizontally. The “horizontal” H's are called “equatorial” and the “vertical” H's are called “axial”.

3) Try to put colored balls into the “axial” positions. Then try to manipulate the model so that the “axial” atoms become “equatorial”, and the “equatorial” atoms become “axial”.

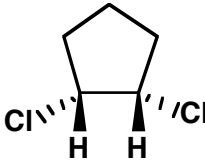
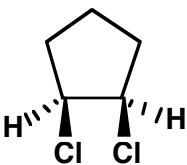
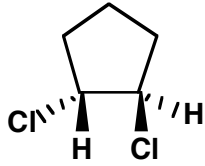
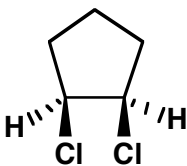
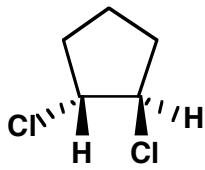
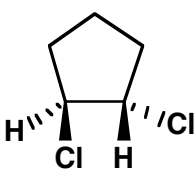
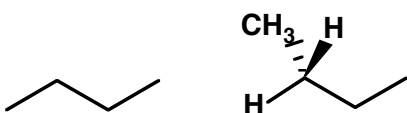
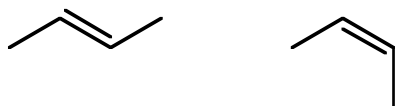
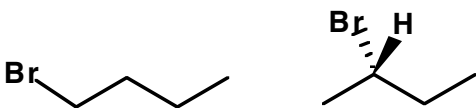
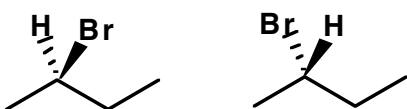
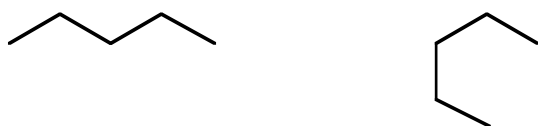
-ask instructor to come over and give you cyclohexane spiel

SAME OR DIFFERENT?

Rules:

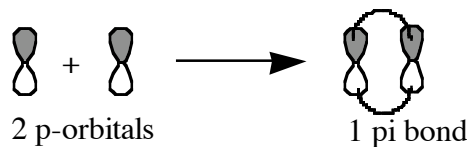
1. Structures which can be interchanged or made equivalent by rotations around single bonds are considered to be the same.
2. “Isomers” are things with the same formula that can't be made superimposable by simple rotations around single bonds.
(not required, but for class will eventually need to be able to distinguish “structural isomers” from “stereoisomers”)

Classify the following pairs as “same” or “isomers”



Orbitals and Pi-Bonds

The models you have built so far have used tetrahedral atoms and two flexible “banana bonds” for making double bonds. From a molecular orbital perspective, it is often more useful to consider a double bond as consisting of a straight sigma bond and a pi-bond made from the overlap of 2 parallel, non-hybridized p-orbitals.



Make a model of ethene, $\text{CH}_2=\text{CH}_2$, using trigonal atoms rather than tetrahedral atoms. The trigonal atoms all have holes in the middle. Poke sticks through the middle to represent p-orbitals.

The following Q's are not for points, but can be helpful for learning.

1. Draw the molecule with the atoms in the plane of the paper, ignoring the p-orbitals at first.
Question: If you were required to draw the p-orbitals, would they be in the plane of the paper, or perpendicular to it?

2. Draw the molecule with the carbons and the p-orbitals in the plane of the paper, ignoring the hydrogens at first. Then add the four hydrogens.

Question: are the atoms in the plane of the paper (drawn with straight lines) or are they not in the plane of the paper (so that they should be drawn with hashes and wedges)?

3. Which picture is easier to draw, the picture in 1 or in 2?

Note: Normally is you want to draw an alkene, you don't draw the p-orbitals, and it's way easier to draw with the atoms all in the plane. You should know there are perpendicular p-orbitals that are **not** in the plane of the atoms are. But you don't draw them.

- But, if you want to draw the orbitals, then you normally do that with the p-orbitals in the paper, in which case the atoms need to be hash/wedged.