MOLECULAR STRUCTURE

For each of the following molecules, make the models and then draw the models, using the hash/wedge/straight-line convention. Use tetravalent atoms. Make double bonds by using two of the soft, flexible white bonds to make "banana double bonds".

- **<u>For molecules involving lone-pairs, draw them with the lone pairs shown</u>**. Use a hash, wedge, or straight-line to show where in 3-D space the lone pair is, and then put a "double-dot" on the end to illustrated that it's a lone-pair rather than an atom.
- **<u>Draw in all hydrogens</u>**. Use a hash, wedge, or straight-line to show where in 3-D space the hydrogen is, and draw an H at the end. (In regular "skeleton structures" H's may be omitted, but for this exercise you need to draw them in to practice and to help understand where they actually sit.)
- **<u>You do not need to write "C" on carbons</u>**. As in regular "skeleton structures", the understanding is that any vertex (or end of stick) is a C unless indicated otherwise. But anything that isn't a carbon (whether H, N, O, Br, or lone-pair) you need to specify.

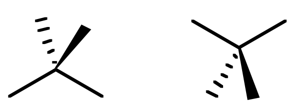
Guidelines for Drawing Models:

A. 3-D Perspective

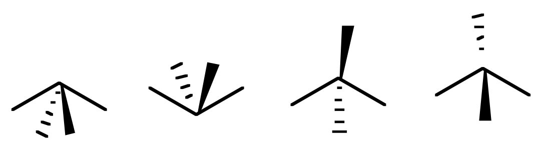
1. Keep as many atoms as possible in a single plane (plane of the paper) by zig-zagging. Connections within the paper are drawn with straight lines.
2. Use wedges to indicate atoms that are in front of the plane.
3. Use hashes to indicate atoms behind the plane.

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 looks tetrahedral
-for polyatomic molecules, <u>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.</u>



Good! Look tetrahedral



Bad! These don' t look tetrahedral!

1. ALKANE. butane, $CH_3CH_2CH_2CH_3$
-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, $CH_3CH_2CH_2CH_2CH_3$

3. HALOALKANE. 2-bromobutane, $CH_3CHBrCH_2CH_3$
-notice that if the 4 carbons are co-planar zig-zagged, the attached Br can't be in the same plane.
-Compare with a partner two structure in which the Br is in front(wedged) in one versus behind (hashed) in the other. Are they the same molecule, or isomers? (Q2 on "same-or-different" page)
-ignore the lone pairs on the Br (in this case)

4. ALKENE. Draw both: a) trans-2-butene, $CH_3CH{=}CHCH_3$
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 2 different orientations, and specify the lone-pairs.
-Draw pictures in which both the oxygen and both the hydrogens 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, CH_3CH_2OH

8. ETHER. Diethyl ether, $CH_3CH_2OCH_2CH_3$

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. CH_3CH_2CHO.

11. KETONE. $CH_3CH_2C(O)CH_2CH_3$.

12. ACID. $CH_3CH_2CO_2H$.

13. ESTER. $CH_3CH_2CO_2CH_3$.

14. AMMONIA. NH_3

15. AMINE. $(CH_3CH_2)_2NH$

16. AMIDE CH_3CONH_2.

17. CYCLIC COMPOUNDS A. Cyclopropane $(CH_2)_3$
-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, $CH_3CH_2CH(CH_3)_2$
-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 "CH_3" 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 $(CH_2)_6$
-Don't bother to draw! Too tough! But do build the model.
1) notice that the 6 carbons do <u>not</u> 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?

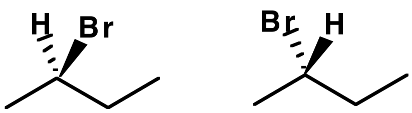
Rules:

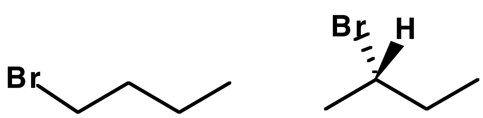
1. Structures which can be interchanged or made equivalent by rotations around single bonds are considered to be the same.
2. "Isomers" are things with the same formula that can't be made superimposable by simple rotations around single bonds.

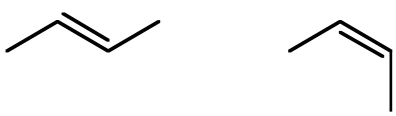
(not required, but for class will eventually need to be able to distinguish "structural isomers" from "stereoisomers")

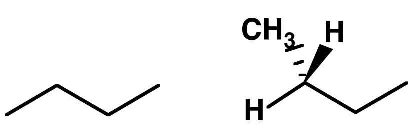
Classify the following pairs as "same" or "isomers"

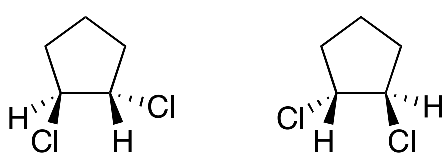
1. 

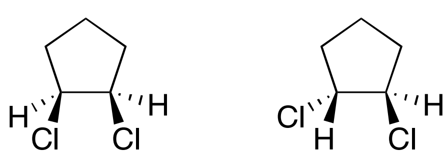
2. 

3. 

4. 

5. 

6. 

7. 

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