4 Targets: 1. 3-D Drawing
2. Condensed formula to Lewis structure
3. Functional Groups
4. Isomers, including structure versus stereoisomers (p 4)

Molecular Structure   1

MOLECULAR STRUCTURE

For each of the following molecules, draw their 3-D structure. You will usually need to have converted the condensed structure into a Lewis structure. Draw in all hydrogens.
- For molecules involving lone-pairs, draw them with the lone pairs shown. While this may not be required for test questions, VSEPR is impacted by lone pairs, so they indirectly impact where atoms are located. For this exercise, try to show where in space the lone pairs will be. To do so, put a "double dot" on the end of a stick (in place), or wedge (in front) or hash (in back).

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, 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.
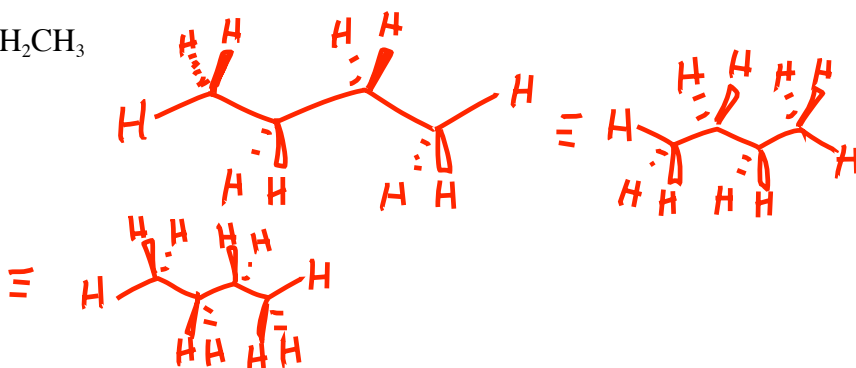

Good! Look tetrahedral   Bad! These don't look tetrahedral!
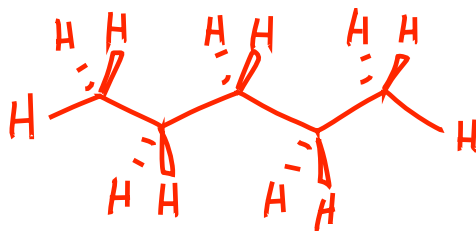
1. ALKANE. butane, $CH_3CH_2CH_2CH_3$
-take the chain and wiggle around all the single bonds.
-The most stable actual shape is the one with the carbons zig-zagged and co-planar.
-Notice the symmetry possible.

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 <u>can't</u> 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?

Isomers, not same
Stereoisomers

nonequal
mirror
image
enantiomers
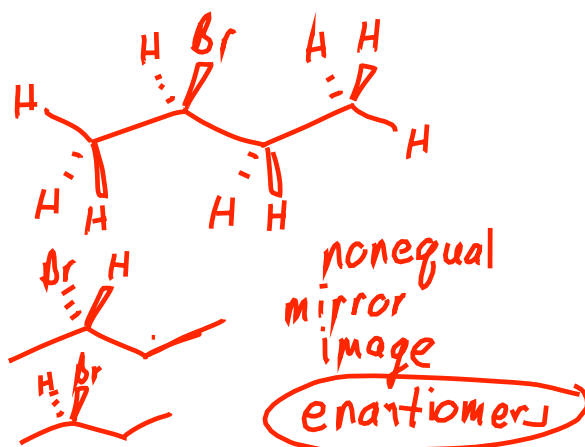
4. ALKENE. Draw both: a) trans-2-butene, $CH_3CH=CHCH_3$
                  and b) cis-2-butene
(trans means the two CH_3 groups are on the opposite sides
of the double bond; cis means they are on same side)
-notice that not only the 2 double-bonded
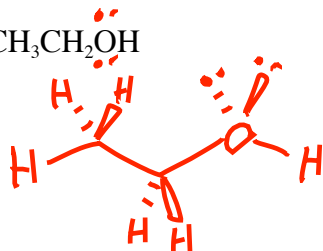C's but also the four atoms directly
attached are all co-planar.

trans

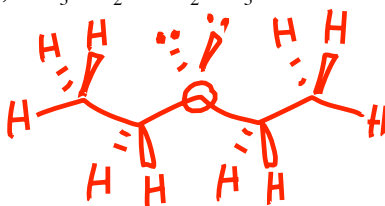*cis*
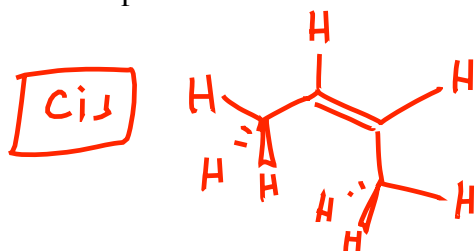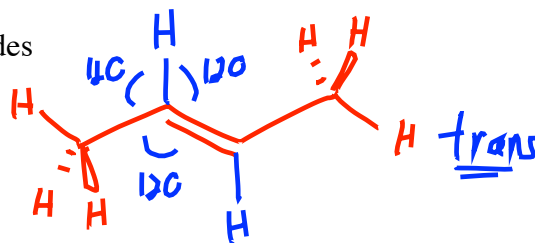
5. ALKYNE. 2-butyne, CH_3CCCH_3
-draw Lewis structure first

linear

show linear, 180°
no zig-zag on
C≡C carbons
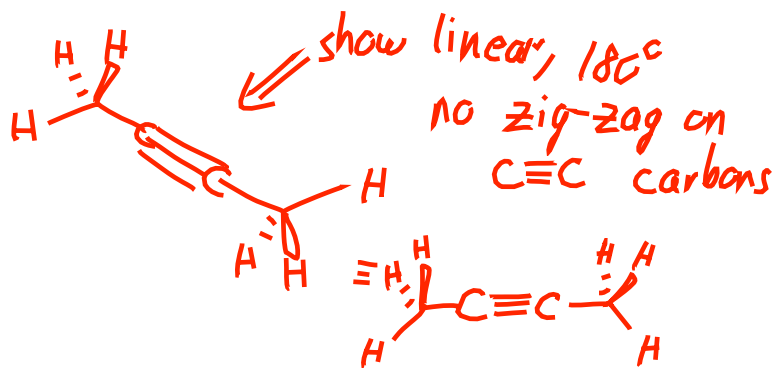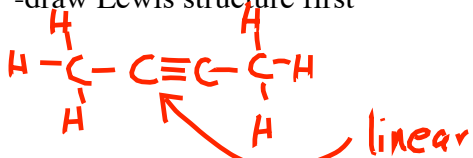
6. WATER. H_2O
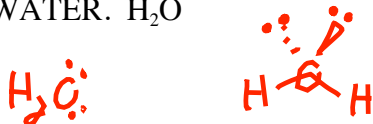
7. ALCOHOL. Ethanol, CH_3CH_2OH
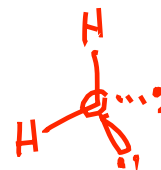
8. ETHER. Diethyl ether, $CH_3CH_2OCH_2CH_3$

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!
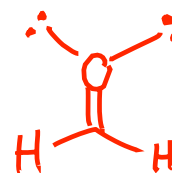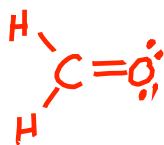
lone pairs in plane

10. ALDEHYDE. CH_3CH_2CHO.
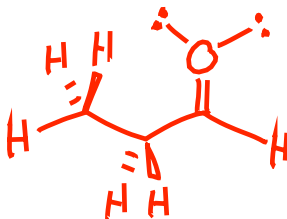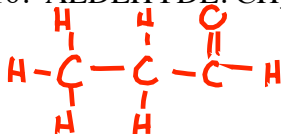
11. KETONE. $CH_3CH_2C(O)CH_2CH_3$.
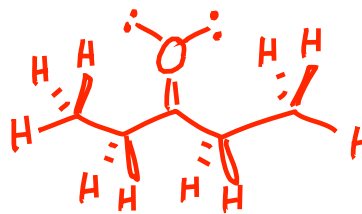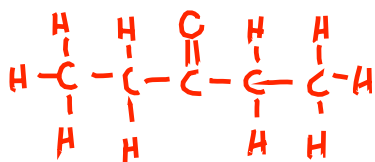
12. ACID. $CH_3CH_2CO_2H$.
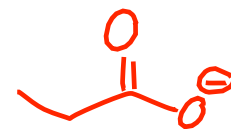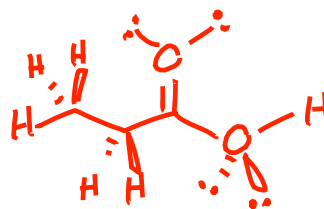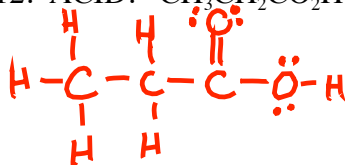
conj anion resonance

13. ESTER. $CH_3CH_2CO_2CH_3$.
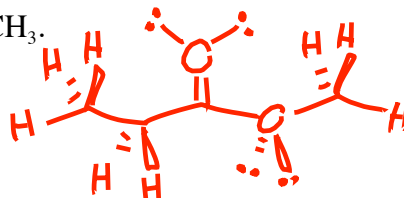
14. AMMONIA. NH_3
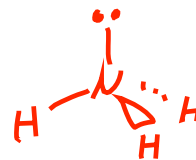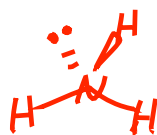
15. AMINE. $(CH_3CH_2)_2NH$
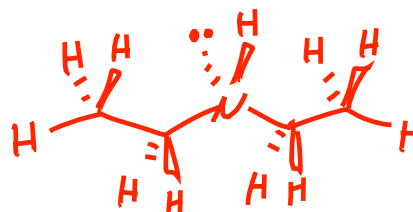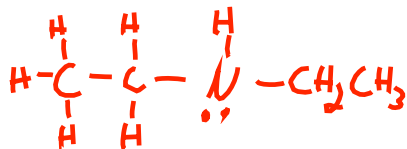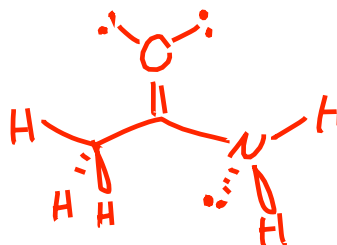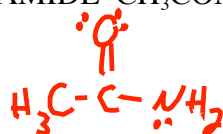
16. AMIDE CH_3CONH_2.

SAME OR DIFFERENT? Classify the following pairs as "same" or "isomers". 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.
 (For class, we will eventually need to be able to distinguish "structural isomers" from "stereoisomers", so try to do that if possible. And within stereoisomers, by test two we'll need to distinguish between "enantiomers", which are mirror image isomers; versus "diastereomers", which are cis/trans isomers.)

enantiomers (mirror image) vs. diastereomers (cis/trans)

same

stereoisomers (enantiomers)
mirror image

$CH_2BrCHCH_2CH_3$

$CH_3CHBrCH_2CH_3$

structural isomers (condensed formulas differ)

$CH_3CHCHCH_3$ *trans*   *cis*

stereoisomers (diasteriomers)

$CH_3CH_2CH_2CH_3$

same

trans   trans

stereo   (mirror)

Cis   trans

stereo   diastereomer

Cis   Cis

same