Key

Sp12

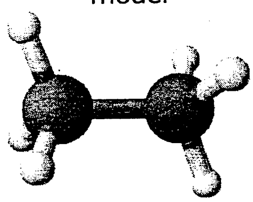
ChemActivity 29

Conformers

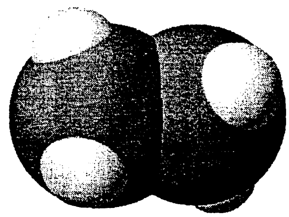
(How and why do molecules "twist?")

Model 1: Representations of ethane in its most favorable conformation

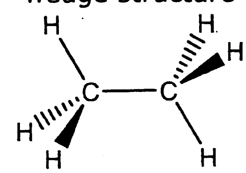
Ball-and-stick model



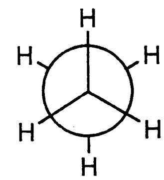
Spacefilling model



Lewis dash-and-wedge structure



Newman projection



Critical Thinking Questions:

1. Each representation in Figure 1 shows ethane (CH_3CH_3) in its lowest potential energy (most favorable) conformation. If you have a model set available, make a model of ethane and rotate the single bonds until it is in this conformation.

   a. Construct an explanation for why this conformation is the most favorable.

   All of the C-H bonds are off-set which minimizes the repulsion of the e⁻'s in these bonds.

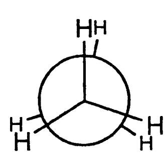
   b. Consider the Newman Projection in Figure 1. What atom is at the center of the picture?

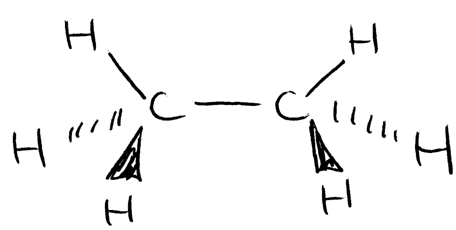
   carbon

   c. The atom you named in CTQ 1b is represented as a large circle or disc. What single atom is hidden from view behind the disc?

   Carbon

2. Consider the Newman projection shown below of ethane in (nearly) its least favorable conformation. If you have a model set available, rotate the single bonds until it is in this conformation. Draw a dash-and-wedge structure for this conformation.





3. In your own words, explain what the term *conformation* means, as applied to ethane.

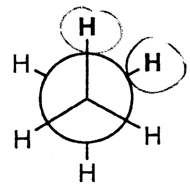
   Conformation means the rotation (movement) of C-C single bonds.

4. Structures that represent the same molecule in different conformations are termed <u>conformers</u>. Construct an explanation for why the conformer in Model 1 is called **staggered** and the conformer in CTQ 2 is called **eclipsed**.

atoms & bonds are off-set (staggered)

atoms & bonds are aligned (eclipsed)

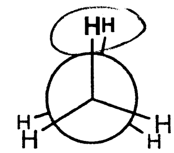
5. Look at your model "end-on" and compare with the Newman projections below. The angle you observe between the hydrogens at the top of each structure in **boldface** is called the torsional angle. Circle the correct torsional angle for each conformer.



staggered

Torsional angle (staggered)

0°
60°
120°
180°



eclipsed

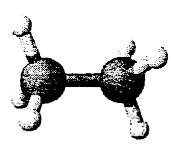
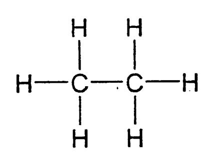
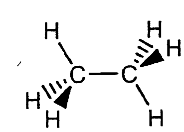
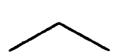
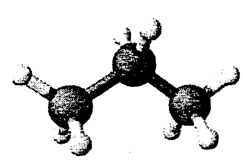
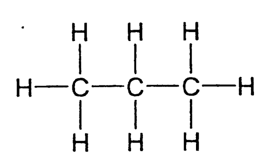
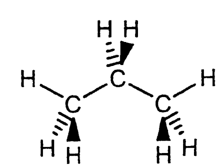
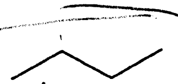
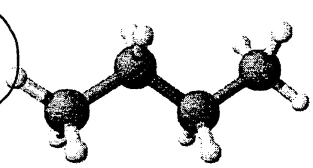
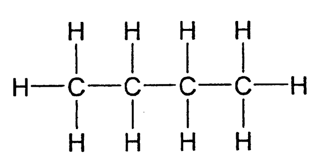
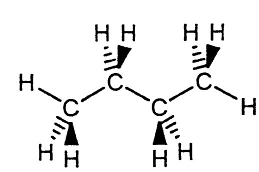
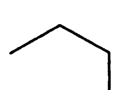
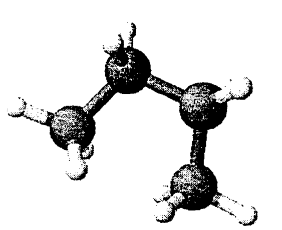
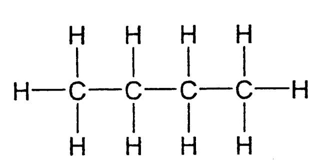
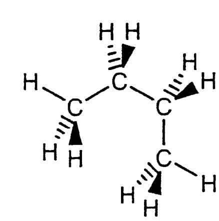
Torsional angle (eclipsed)

0°
60°
120°
180°

6. What repulsive forces will cause ethane in the eclipsed conformation to quickly adopt the staggered conformation?

electrostatic repulsion of the C-H single bonds

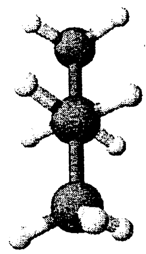
Model 2: Some representations of alkanes with 2, 3 and 4 carbons

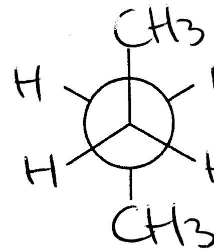
Skeletal or "Stick" structure	Ball-and-stick structure	Lewis structure	Dash-and-wedge structure
ethane			
 propane			
 butane			
 butane			

Critical Thinking Questions:

7. Underneath each stick structure in Model 2, write the name of the alkane. see previous page

8. The ball-and-stick structure below matches one of the two butane conformations shown in Model 2, looking "end-on" down the bond between carbons 2 and 3. Circle the stick structure in Model 2 that matches the structure below.



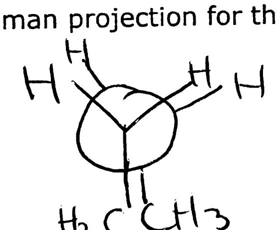


9. Complete the Newman projection at the right in CTQ 7 by adding H or CH_3 groups so that it represents the conformation shown in the ball-and-stick structure at the left.

10. Consider the <u>other</u> stick structure for butane in Model 2 (the one you did <u>not</u> circle in CTQ 7), sighting down the C2–C3 bond.

   a. Is this structure **staggered** or **eclipsed** (circle one)? You may use your model to help you.

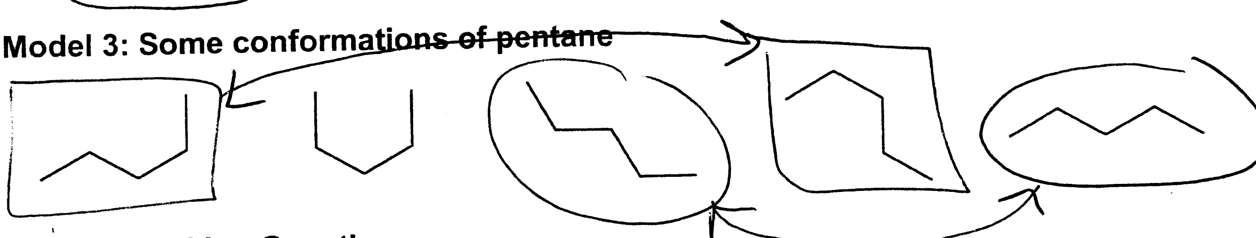
   b. Draw a Newman projection for this conformation of butane.



   c. At room temperature, the single bonds in butane are continually rotating through the staggered and eclipsed conformations. However, the molecule spends more time closer to one of the two extremes. Which conformation is it likely to spend more time in—

   staggered or **eclipsed** (circle one)?

Model 3: Some conformations of pentane



Critical Thinking Questions:

11. Circle the two structures of pentane in Model 3 that are in their most favorable conformation. Explain why these are the most favorable.

Because they are staggered

12. Draw a line to connect the two structures that you circled in Model 3. These two structures are in the same conformation, but the molecule as a whole is rotated.

see above

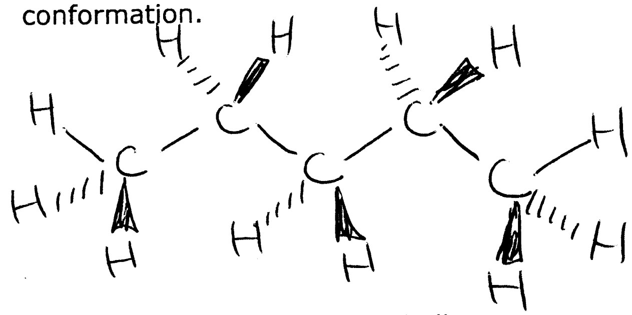
boxed

13. Find two other structures in Model 3 that are identical (*i. e.,* in the same conformation), and draw a second line to connect them. see previous page

14. What is the total number of distinct conformers of pentane shown in Model 3? 3

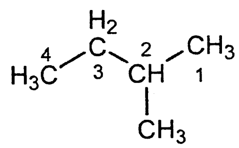
Exercises:

1. Draw a wedge and dash-bond representation of pentane in its most favorable conformation.

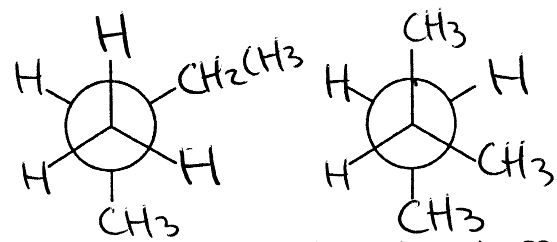


2. Consider the molecule 2-methylbutane.

   a. Using the templates at the right, complete two staggered Newman projections for 2-methylbutane: one sighting down the C1–C2 bond and the second sighting down the C2–C3 bond.

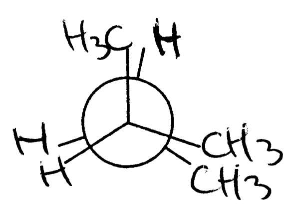


C1-C2

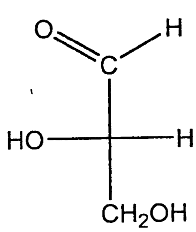


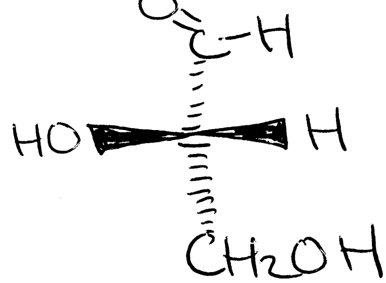
C2-C3

   b. Complete the eclipsed Newman projection for 2-methylbutane sighting down the C2–C3 bond.



3. Sugars and other complex molecules are often depicted using a representation called a Fisher projection. In a Fisher projection all <u>horizontal</u> bonds are assumed to come out of the page toward you (wedge bonds) and all <u>vertical</u> bonds are assumed to go back into the page, away from you (dash bonds). Draw a wedge and dash representation of the Fisher projection of glyceraldehyde shown below.



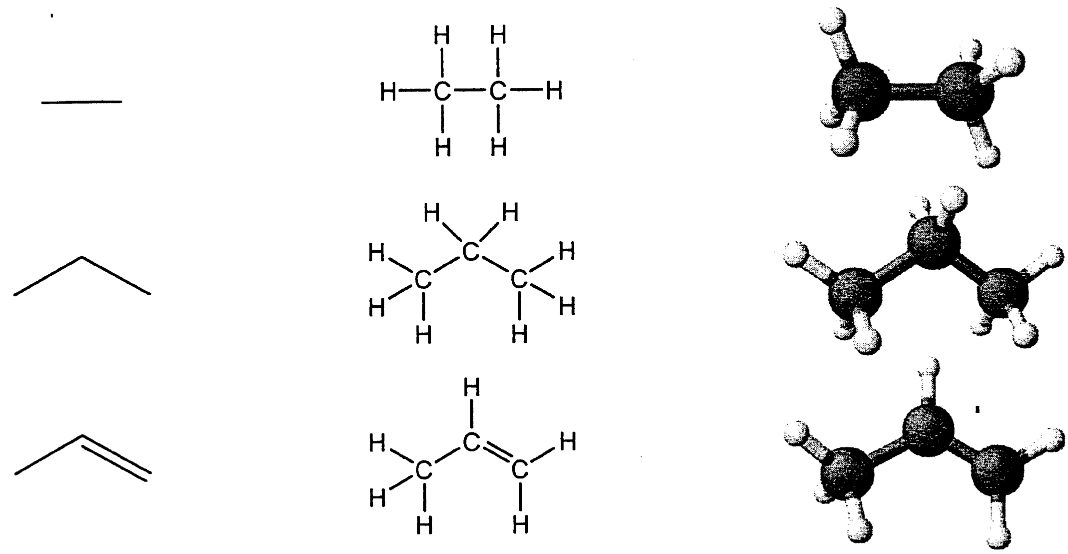


Constitutional and Geometric Isomers

(Are they identical, or are they isomers?)

Model 1: Representations of some organic molecules

Skeletal or "Stick" structure	Lewis structure	Ball-and-stick structure



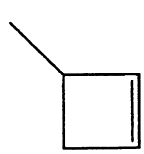
Critical Thinking Questions:

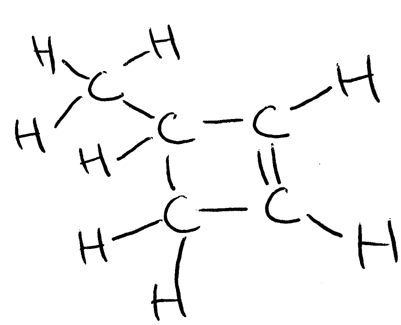
1. Consider the Lewis structures in Model 1. How many covalent bonds does each carbon have? 4

2. In skeletal representations, the hydrogens are not shown. Explain how it is still possible to tell how many hydrogens there are on each carbon.

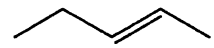
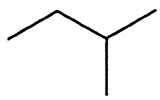
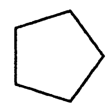
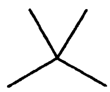
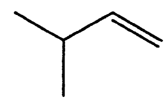
   We add H's to give each Carbon 4 bonds.

3. Draw a Lewis structure representation of the molecule for which a skeletal representation is shown below.





Model 2: Constitutional Isomers

Column 1		Column 2	
structure	molecular formula	structure	molecular formula
	C_5H_{12}		C_5H_{10}
	C_5H_{12}		C_5H_{10}
	C_5H_{12}		C_5H_{10}

Critical Thinking Questions:

4. Complete Model 2 by writing in the missing molecular formulas in both columns. see above
5. What do the molecules in a given column (1 or 2 in Model 2) have in common with the other molecules in that column?

   same molecular formula

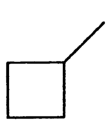
6. What do the molecules in a given column **not** have in common with the other molecules in that column?

   different connections btwn atoms

7. All the structures in a given column are <u>constitutional isomers</u> of one another, but the structures in Column 1 are not constitutional isomers of structures in Column 2. Based on this information, write a definition for the term <u>constitutional isomers</u>.

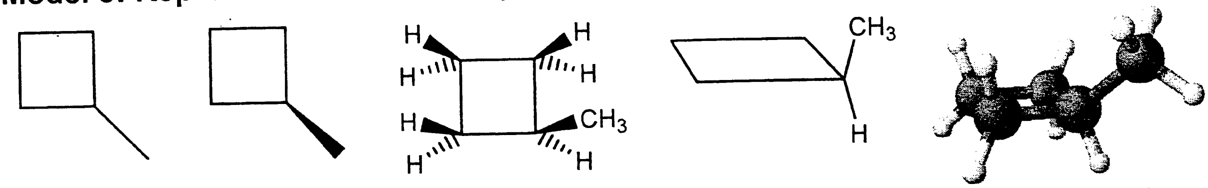
   Cpds w/ the same molecular formula, but different atomic connections,

8. If the molecule shown below were placed into Model 2, would it belong in **Column 1** or **Column 2** (circle one)? Explain your choice.



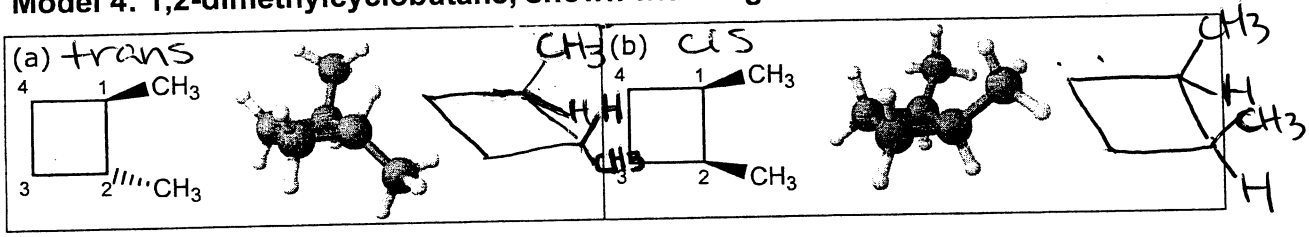
column 2 b/c the molecular formula is C_5H_{10}

Model 3: Representations of methylcyclobutane



Skeletal ("stick")	Wedge and dash	Wedge and dash with explicit hydrogens	Perspective	Ball-and-stick

Model 4: 1,2-dimethylcyclobutane, shown with ring carbons numbered 1–4



Critical Thinking Questions:

9. Are the molecules in boxes (a) and (b) of Model 4 constitutional isomers of each other? Explain.

   No, the connections & molecular formula are the same.

10. *Other than bonds to carbons within the ring*, what two groups are bonded to the following carbons?
    a. carbon 1 in box (a)? H & CH_3
    b. carbon 1 in box (b)? H & CH_3
    c. carbon 2 in box (a)? H & CH_3
    d. carbon 2 in box (b)? H & CH_3

11. If you have access to a model kit, make models of the two molecules in Model 4 (C = black; H = white; use the short bonds for single bonds). Is it possible to rotate single bonds in the models such that the molecule in box (a) is the same as the one box (b)?

    No

Information:

Since each carbon in the molecule in box (a) in Model 4 is bonded to the same four groups as the corresponding carbon in the molecule in box (b), the molecules are said to have the same **connectivity**.

You confirmed in CTQ 11 that the two structures of 1,2-dimethylcyclobutane shown above are not simply **conformers** of each other.

Imagine that the four carbons of the cyclobutane ring define a plane. In one structure, the two methyl groups are on the *same side* of this plane, and in the other they are on *opposite sides* of the plane. The single bonds in the ring cannot rotate without breaking the ring. Two groups on the *same side* of the plane are considered to be *cis* to one another. Groups on opposite sides are called *trans*.

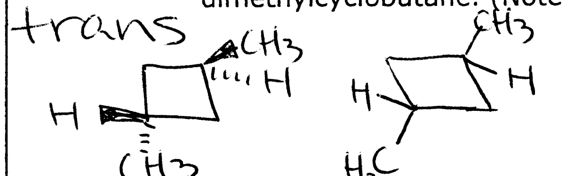
Geometric isomers (*cis-trans* isomers) are molecules that have the same connectivity and differ only in the geometric arrangement of groups.

Critical Thinking Questions:

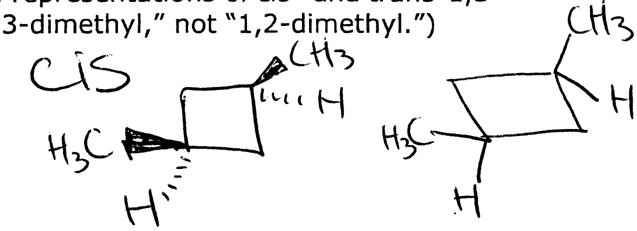
12. Label one box in Model 4 with the name "*cis*-1,2-dimethylcyclobutane" and the other with the name "*trans*-1,2-dimethylcyclobutane." Then add perspective representations into each box. See previous pg

13. Draw wedge-and-dash and perspective representations of *cis*- and *trans*-1,3-dimethylcyclobutane. (Note: that is "1,3-dimethyl," not "1,2-dimethyl.")

trans



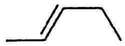
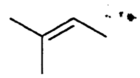
cis

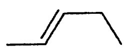
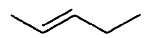


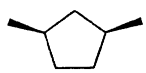
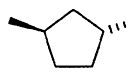
Exercises:

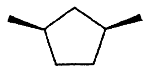
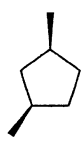
1. Indicate if the following pairs of structures are *identical*, *conformers*, *geometric isomers*, *constitutional isomers*, or *not isomers*.

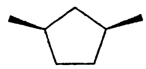
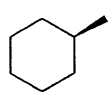
   a. 1,2-dimethylcyclobutane and 1,3-dimethylcyclobutane — constitutional isomers

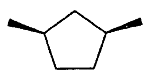
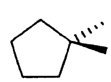
   b.  and  const. isomers

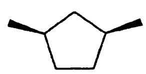
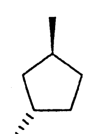
   c.  and  conformers

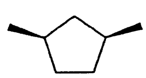
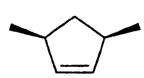
   d.  and  geometric isomers

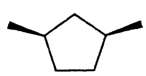
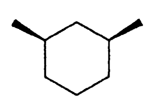
   e.  and  identical

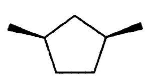
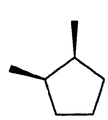
   f.  and  constit. isomers

   g.  and  constit. isomers

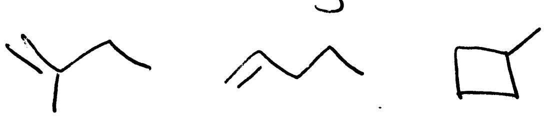
   h.  and  geometric isomers

   i.  and  not isomers

   j.  and  not isomers

   k.  and  constitut. isomers

2. Draw a structure for a molecule not shown in this activity that would belong in Column 2 of Model 2. many answers possible



Isomers

(What are some different types of isomers?)

Information: Review of some types of isomers, from least to most similar

1. **Constitutional isomers**: molecules with the same molecular formula but different structures (different connectivity).
2. **Geometric isomers** (*cis-trans* isomers): molecules that have the same connectivity and differ only in the geometric arrangement of groups.
3. **Conformational isomers** (conformers): molecules that can be interconverted by rotation around single bonds.

Model 1: Alkenes

As we saw in ChemActivity 21, there is no free rotation around double bonds at room temperature. This means the two molecules below are not the same, as they cannot be interconverted *via* rotation of single bonds.

trans cis

Critical Thinking Questions:

1. Recall the meanings of the terms *cis* and *trans* as applied to cycloalkanes. By analogy, label one of the molecules in Model 1 "*cis*-2-butene" and the other "*trans*-2-butene." see above
2. According to the definitions in the Information, what is the relationship between *cis*-2-butene and *trans*-2-butene?
   cis & trans represent geometric isomers of a cpd.
3. Draw skeletal ("stick") representations of *cis* and *trans*-2-butene.

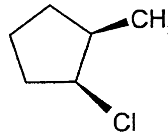
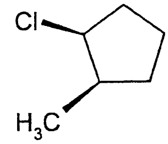
trans cis

4. Draw skeletal ("stick") representations of *cis* and *trans*-3-hexene.

trans cis

5. Identify the type of isomeric relationship between each pair of molecules below, from the following five choices (arranged from least to most similar): *not isomers, constitutional isomers, geometric isomers, conformers, identical.*

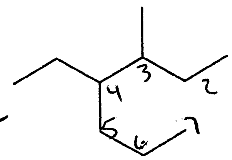
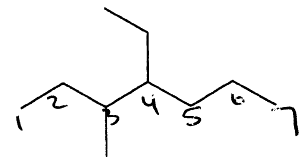
a.

 and 

identical

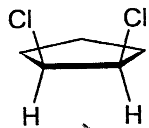
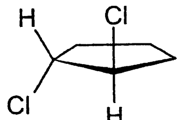
b.

both cpds 4-ethyl-3-methyl heptane

 and 

conformers

c.

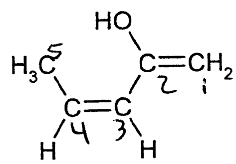
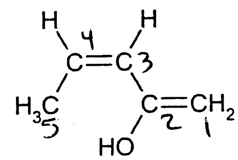
 and 

cis trans

geometric isomers

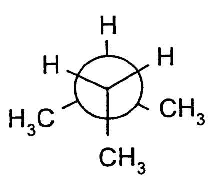
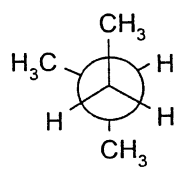
d.

both cis

 and 

identical

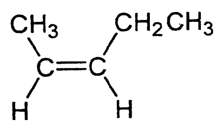
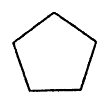
e.

 and 

conformers

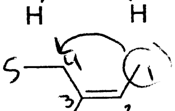
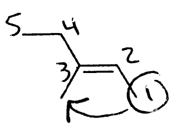
f.

both C_5H_{10}

 and 

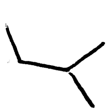
constitutional isomers

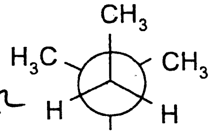
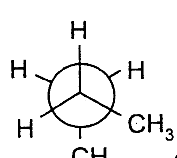
* g.

 and 

geometric isomers

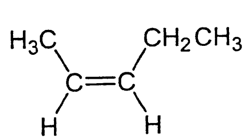
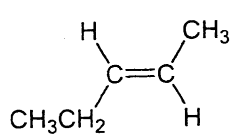
h.



C_5H_{12}  and  C_4H_{10}

not isomers

i.

 and 

cis trans

geometric isomers

* We cannot use cis & trans for these 2 cpds. We need E & Z — not covered in our class.

Exercises:

1. Redraw the structures from CTQ 5b as condensed structures.

2nd cpd (on Rt) $CH_3CH_2CH(CH_3)CH(CH_2CH_3)CH_2CH_2CH_3$

1st cpd (on Left) $CH_3CH_2CH(CH_2CH_2CH_3)CH(CH_3)CH_2CH_3$

2. Redraw the structures from CTQ 5e as condensed structures.

1st cpd (on Left) $CH_3CH_2CH(CH_3)_2$

2nd cpd (on Rt) $CH_3CH_2CH(CH_3)_2$

3. Redraw the structures from CTQ 5g as condensed structures.

C=C double bond can be shown.

1st cpd (on Left) $CH_3CH_2C(CH_3)CHCH_3$

2nd cpd (on Rt). $CH_3CH_2C(CH_3)CHCH_3$

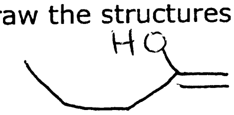
4. Redraw the structures from CTQ 5h as condensed structures.

1st cpd (on Left) $CH_3CH_2CH(CH_3)_2$

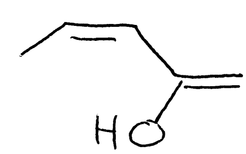
2nd cpd (on Rt) $CH_3CH_2CH_2CH_3$

5. Redraw the structures from CTQ 5d as skeletal ("stick") structures.

1st cpd (on Left)

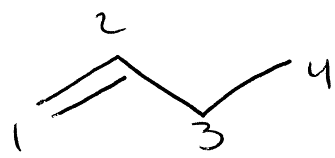


2nd cpd (on Rt)



6. Name the molecules in CTQ 5abceh.
   a. cis-1-chloro-2-methyl cyclopentane
   b. 4-ethyl-3-methyl heptane
   c. cis-1,2-dichloro cyclopentane (cpd on Left)
      trans-1,2-dichloro cyclopentane (cpd on Right)
   e. 2-methyl butane
   h. cpd on Left
      2-methyl butane
      cpd on Right
      butane

7. Draw a representation (any style) of 1-butene. Can this molecule have *cis* and *trans* isomers? If not, explain. If so, draw them.



no cis/trans possible b/c Carbon-1 is bonded to 2 H's.