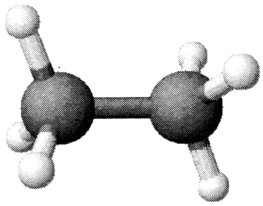
Conformers

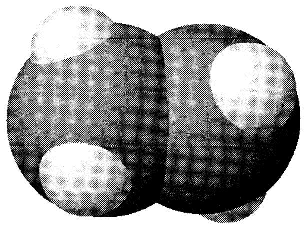
(How and why do molecules "twist?")

Model 1: Representations of ethane in its most favorable conformation

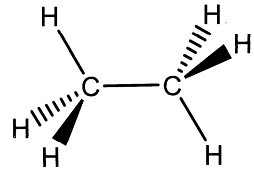
Ball-and-stick model



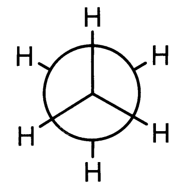
Spacefilling model



Lewis dash-and-wedge structure



Newman projection



Critical Thinking Questions:

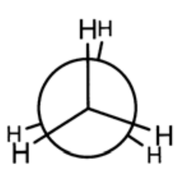
1. Each representation in Figure 1 shows ethane (CH_3CH_3) in its lowest potential energy (most favorable) conformation. If you have a model set available, make a model of ethane and rotate the single bonds until it is in this conformation.

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

   b. Consider the Newman projection in Model 1. What atom is at the center of the diagram?

   c. Consider the Newman projection in Model 1. What atom is represented by the large circle or disc?

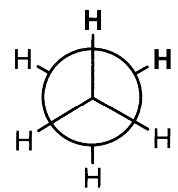
2. Consider the Newman projection shown below of ethane in (nearly) its least favorable conformation. If you have a model set available, rotate the single bonds until it is in this conformation. Draw a dash-and-wedge structure for this conformation.



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

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**.

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

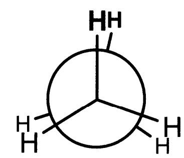
Torsional angle (staggered)

0°

60°

120°

180°



eclipsed

Torsional angle (eclipsed)

0°

60°

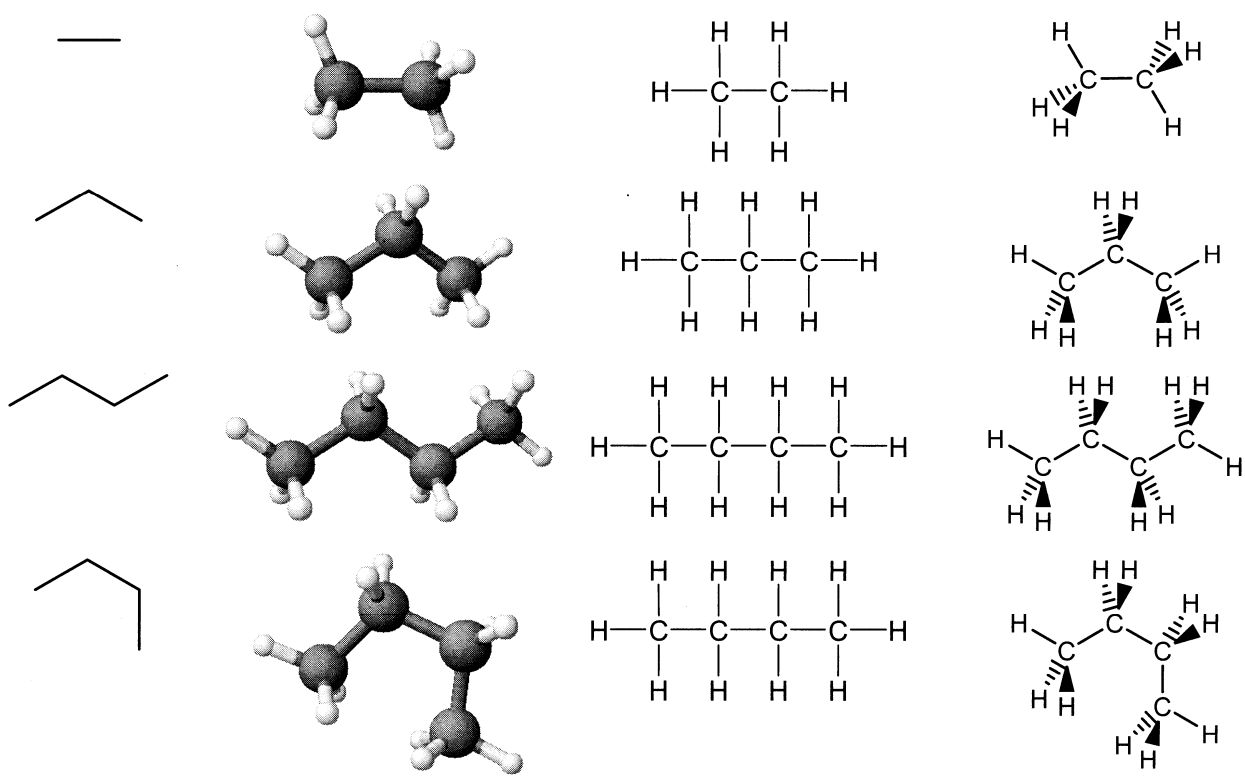
120°

180°

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

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

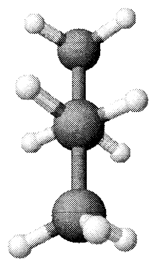
Skeletal or "Stick" structure	Ball-and-stick structure	Lewis structure	Dash-and-wedge structure

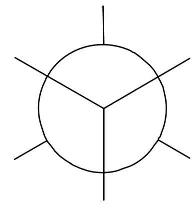


Critical Thinking Questions:

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

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.

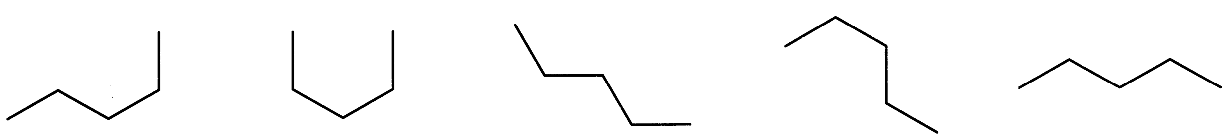
    a. Is this structure **staggered** or **eclipsed** (circle one)? You may use your model to help you.

    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.

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.

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.

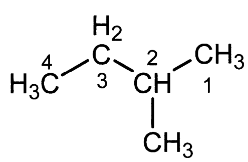
14. What is the total number of distinct conformers of pentane shown in Model 3?

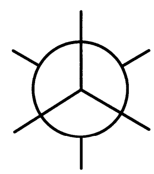
Exercises:

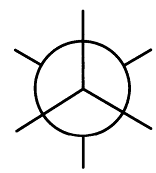
1. Draw a wedge and dash-bond representation of pentane in its most favorable conformation.

2. Consider the molecule 2-methylbutane.

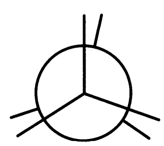
   a. Using the templates at the right, complete two staggered Newman projections for 2-methylbutane: one sighting down the C1–C2 bond and the second sighting down the C2–C3 bond.



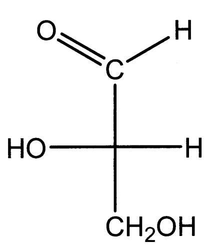




   b. Complete the eclipsed Newman projection for 2-methylbutane sighting down the C2–C3 bond.



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.

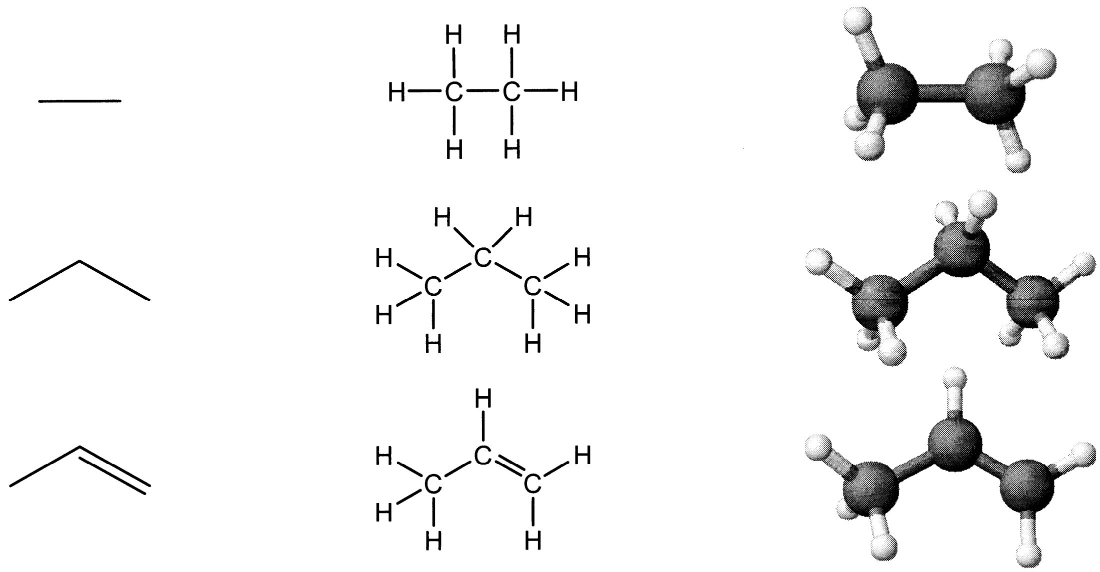


Constitutional and Geometric Isomers

(Are they identical, or are they isomers?)

Model 1: Representations of some organic molecules

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

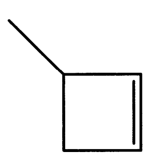


Critical Thinking Questions:

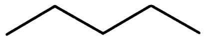
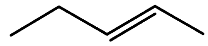
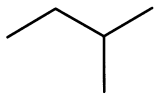
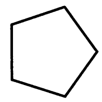
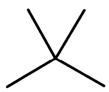
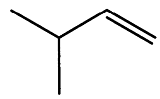
1. Consider the Lewis structures in Model 1. How many covalent bonds does each carbon have?

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.

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

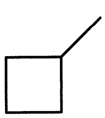


Model 2: Constitutional Isomers

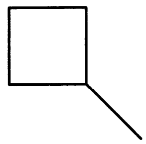
Column 1		Column 2	
structure	molecular formula	structure	molecular formula
	C_5H_{12}		
			
			

Critical Thinking Questions:

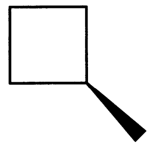
4. Complete Model 2 by writing in the missing molecular formulas in both columns.
5. What do the molecules in a given column (1 or 2 in Model 2) have in common with the other molecules in that column?
6. What do the molecules in a given column **not** have in common with the other molecules in that column?
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>.
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.



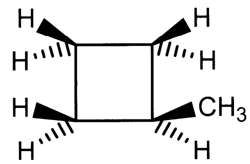
Model 3: Representations of methylcyclobutane



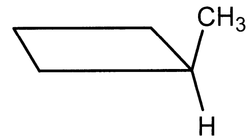
Skeletal ("stick")



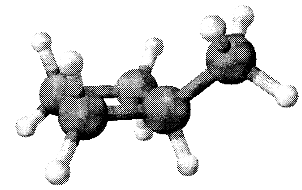
Wedge and dash



Wedge and dash with explicit hydrogens



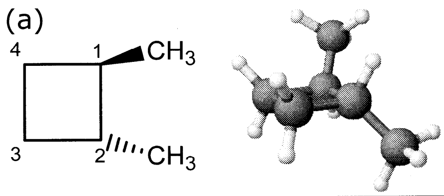
Perspective



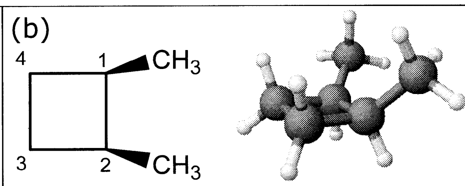
Ball-and-stick

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

(a)



(b)



Critical Thinking Questions:

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

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

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)?

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:

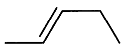
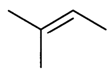
12. Label one box in Model 4 with the name "*cis*-1,2-dimethylcyclobutane" and the other with the name "*trans*-1,2-dimethylcyclobutane." Then add perspective representations into each box.

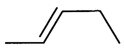
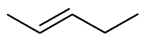
13. Draw wedge-and-dash and perspective representations of *cis*- and *trans*-1,3-dimethylcyclobutane. (Note: that is "1,3-dimethyl," not "1,2-dimethyl.")

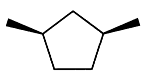
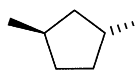
Exercises:

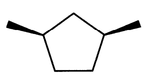
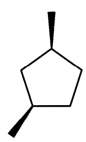
1. Indicate if the following pairs of structures are *identical*, *conformers*, *geometric isomers*, *constitutional isomers*, or *not isomers*.

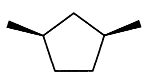
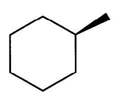
   a. 1,2-dimethylcyclobutane and 1,3-dimethylcyclobutane

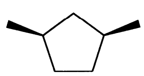
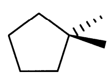
   b.  and 

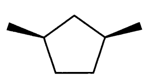
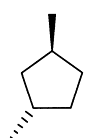
   c.  and 

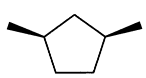
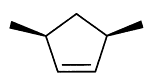
   d.  and 

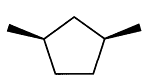
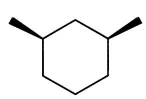
   e.  and 

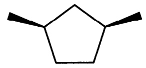
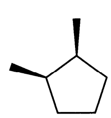
   f.  and 

   g.  and 

   h.  and 

   i.  and 

   j.  and 

   k.  and 

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

Isomers

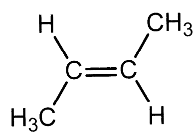
(What are some different types of isomers?)

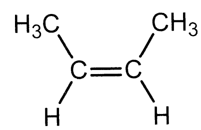
Information: Review of some types of isomers, from least to most similar

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.



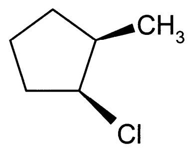


Critical Thinking Questions:

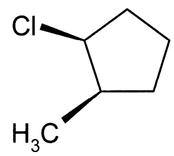
1. Recall the meanings of the terms *cis* and *trans* as applied to cycloalkanes. By analogy, label one of the molecules in Model 1 "*cis*-2-butene" and the other "*trans*-2-butene."
2. According to the definitions in the Information, what is the relationship between *cis*-2-butene and *trans*-2-butene?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

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*.

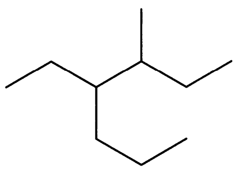
a.



and



b.



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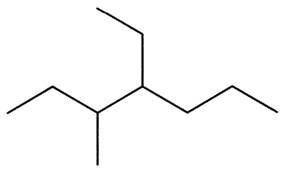
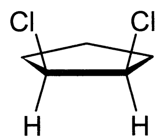


c.



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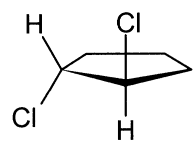
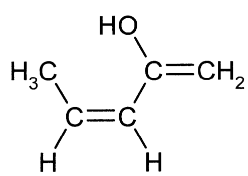


d.



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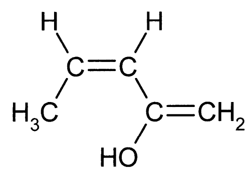
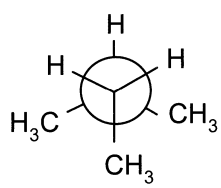


e.



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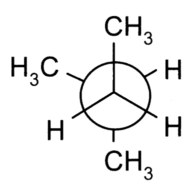
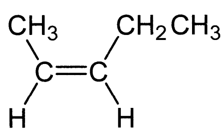


f.



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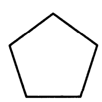
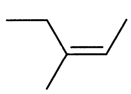


g.



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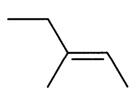
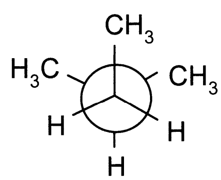


h.



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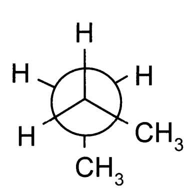
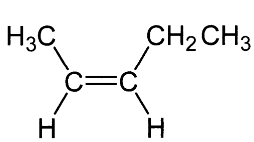


i.



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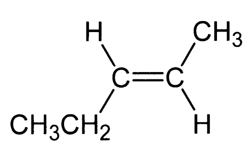

Exercises:

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

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

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

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

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

6. Name the molecules in CTQ 5abceh.

   a.

   b.

   c.

   e.

   h.

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