Discovering Molecular Models #1:
Constitutional Isomers and Conformations of Alkanes & Cycloalkanes

There are no additional tutorial or laboratory notes. Read and bring your course notes, as they provide all of the background material necessary to perform these exercises and problems.

Based on the name of this exercise (Discovering Molecular Models), what else should you bring?

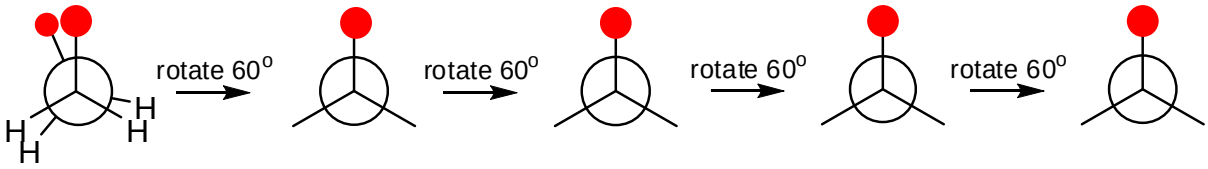
There will be a quiz at the end of this exercise. If you are performing this in the lab, the will count towards your lab component of the course. Likewise, if you are performing this in the tutorial room, it will count towards the tutorial component.

A. Familiarization with Molecular Models

1. Build molecular models of $CH_3CH_2CH_2CH_3$ (butane) and $H_2C{=}CHCH_2CH_3$ (butene). Compare the rotation around the carbon-carbon single bonds to that of the C=C by twisting around the bonds between C1-C2, C2-C3 and C3-C4.

   Explain your observations using the hybridization of each C atom in the molecules.

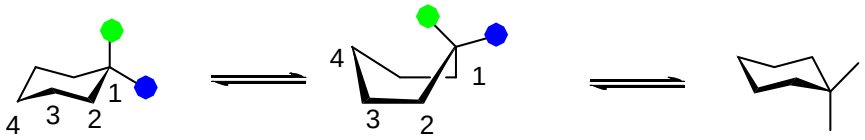
2. Build the molecular model of 1,2-dichloroethane, Cl-CH_2-CH_2-Cl. Use red balls to represent the chlorine atoms. The first Newman project seen looking down the C-C bond is shown. Complete the remaining Newman projections, showing the eclipsed, staggered, and gauche conformations obtained by rotating the *back* carbon by 60° each turn.



eclipsed

   Draw the corresponding energy diagram, similar to the one shown in the notes for butane.

3. Make a model of cyclohexane and put it in the chair conformation. At carbon 1, label the axial position with a green ball and the equatorial position with a blue ball. Convert your chair form to the boat form, and then to the second chair form.



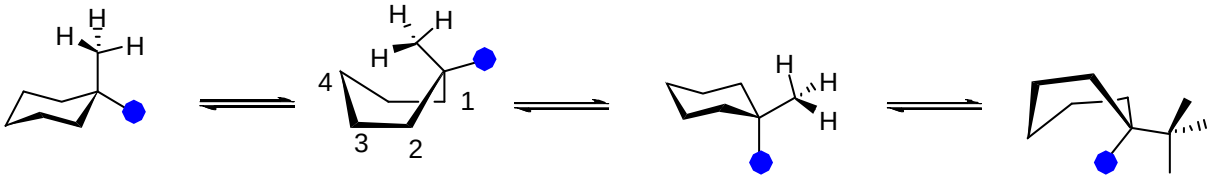
What position does the blue ball occupy in the second chair?

Using the boat form, look down the C2-C3 axis as you would for a Newman projection. What is the conformation you see, staggered or eclipsed? Repeat for the C1-C2 axis.

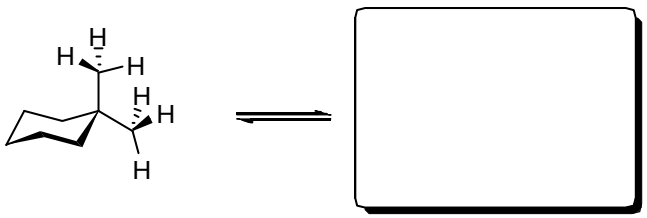
Using either chair form, look down the C2-C3 axis as you would for a Newman projection. What is the conformation you see, staggered or eclipsed? Repeat for the C1-C2 axis.

Which conformation is the most stable?

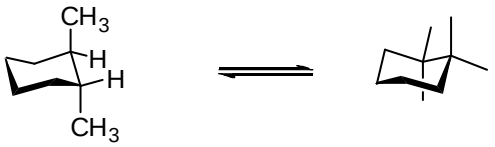
4. Using the same model as above, replace one of the colored balls with another tetrahedral group (a methyl group). You have now made 1-methylcyclohexane. Compare the two chair and the two boat conformations. Which appears to be the least hindered and most stable? Rank the four conformations in terms of their relative stability.



5. Using the same model as above, remove the colored ball and replace it with another methyl group. Draw and compare the two chair forms of this molecule.

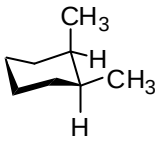


6. Continue using the two methyl groups, and make the model where the two methyl groups are on adjacent carbons (1,2-dimethylcyclohexane). Make both the *trans* and the *cis* forms separately. For each, compare the stabilities of the two chair forms. Are they the same or different? Rank the relative stability of *cis* versus *trans.*

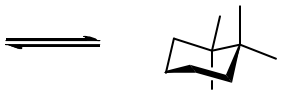


1,2-*trans*

label where the CH_3 groups are in the other chair form.

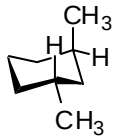


1,2-*cis*

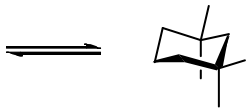


label where the CH_3 groups are in the other chair form.

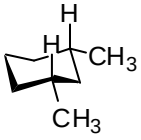
7. Now, place the two methyl groups on carbons 1 and 3, giving 1,3-dimethylcyclohexane. Make both the *trans* and the *cis* forms separately. For each, compare the stabilities of the two chairs. Are they the same or different? Rank the relative stability of *cis* versus *trans.*



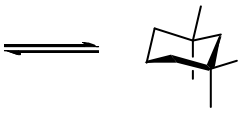
1,3-*trans*



label where the CH_3 groups are in the other chair form.

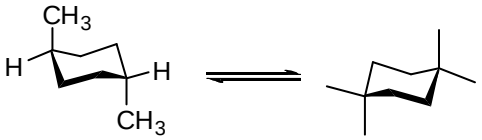


1,3-*cis*



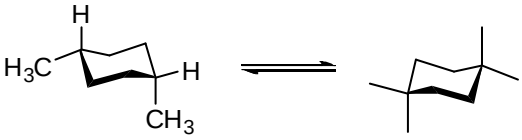
label where the CH_3 groups are in the other chair form.

8. Finally, put the two methyl groups on carbons 1 and 4 (1,4-dimethylcyclohexane). Make both the *trans* and the *cis* forms separately. For each, compare the stabilities of the two chair forms. Are they the same or different? Rank the relative stability of *cis* versus *trans.*



label where the CH_3 groups are in the other chair form.

1,4-*trans*



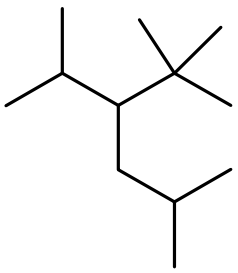
label where the CH_3 groups are in the other chair form.

1,4-*cis*

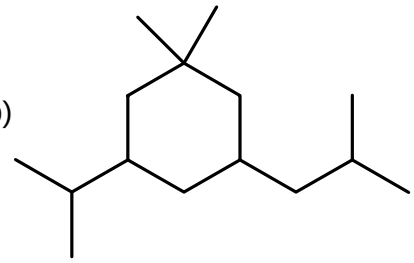
B. Constitutional Isomers, Functional Groups and Intermolecular Forces

9. Classify each carbon as 1°, 2°, 3°, or 4°.

(a)



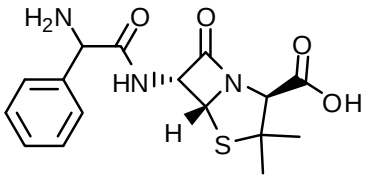
(b)



10. Draw the nine constitutional isomers having the molecular formula C_7H_{16}.

11. Circle and name each functional group in the molecules below. These are taken from your lecture notes. Also be sure you can identify the hybridization of each atom (*sp*, sp^2, or sp^3).

(a)



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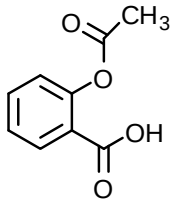

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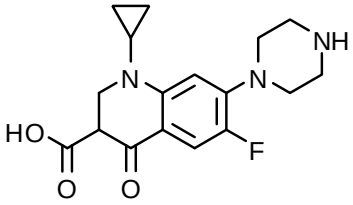

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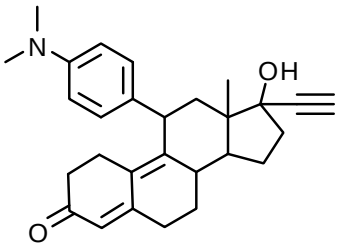

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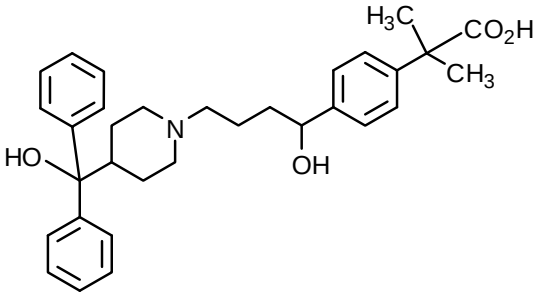

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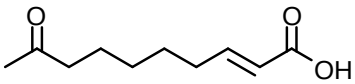

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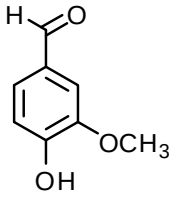
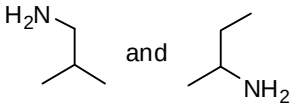
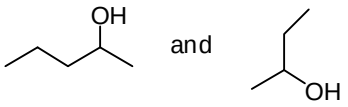
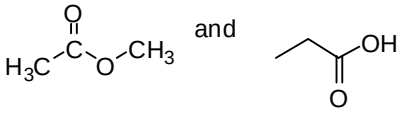
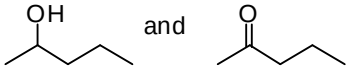


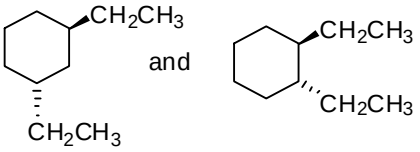
12. Classify each pair of compounds as constitutional isomers, stereoisomers, identical molecules, or not isomers of each other.

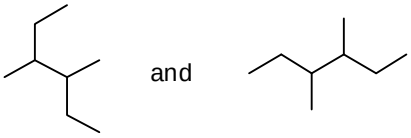
(a) 

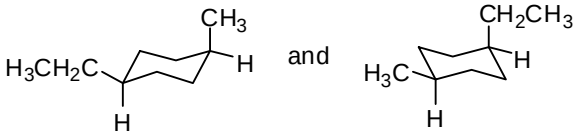
(b) 

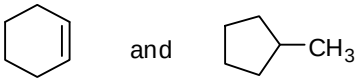
(c) 

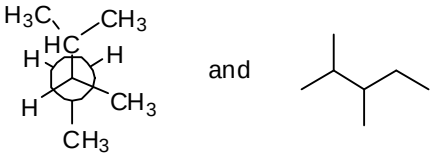
(d) 

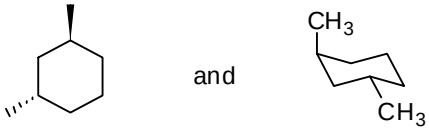
(e) 

(f) 

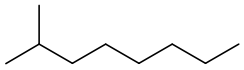
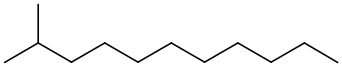
(g) 

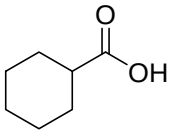
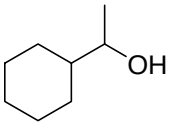
(h) 

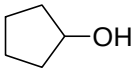
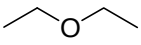
(i) 

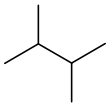
(j) 

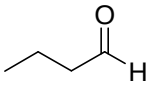
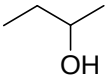
13. For each pair, explain which compound has the higher boiling point.

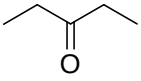
(a)  and 

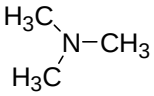
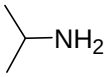
(b)  and 

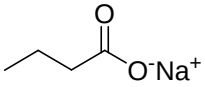
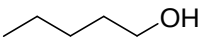
(c)  and 

(d)  and 

(e)  and 

(f)  and 

(g)  and 

(h)  and 

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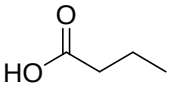
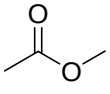
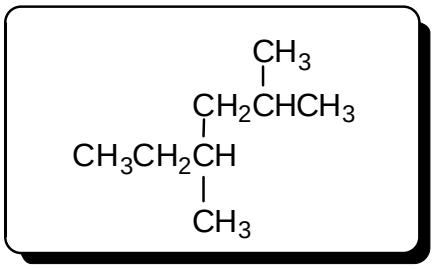
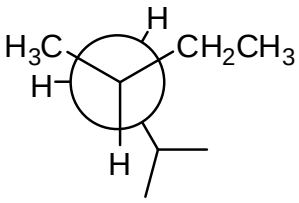
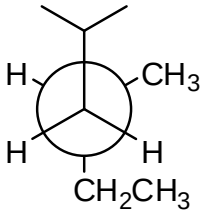
(j)  and 

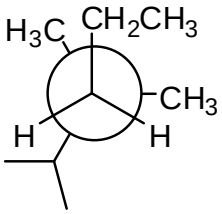
C. Alkane Conformations and Newman Projections

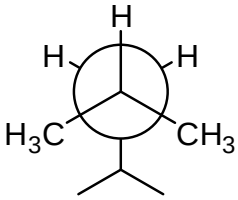
14. Which Newman projection(s) is/are not a representation of the molecule in the box?

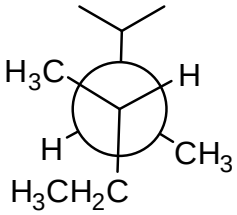




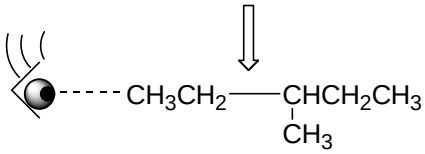






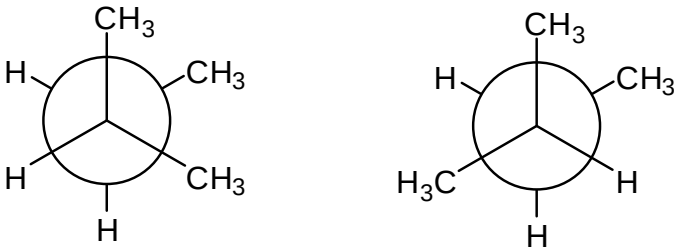


15. Using Newman projections that look from the direction indicated, draw all staggered and eclipsed conformations that result from rotation around the indicated bond.

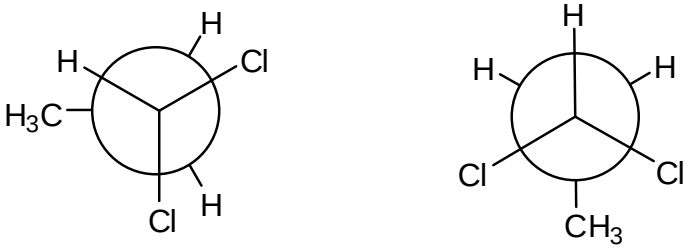


16. Which conformer in each pair is higher in energy? Why?

(a)

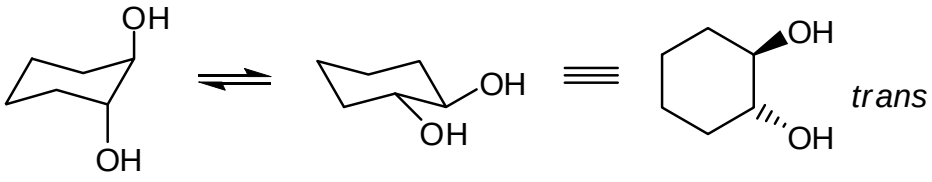


(b)

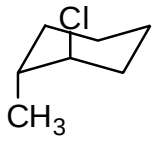


D. Conformations of Cycloalkanes and their Geometric Isomers

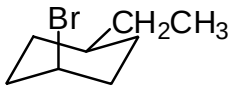
17. For each of the following cyclohexane derivatives, indicate (i) whether the molecule is a *cis* or a *trans* isomer; (ii) whether or not it is shown in its most stable conformation; (iii) draw a representation of the other chair conformation; and (iv) translate each structure to a representation of a flat cyclohexane (hexagon), using dashes and wedges to indicate the groups above and below the ring. Example:

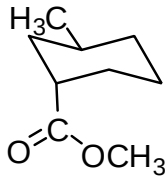


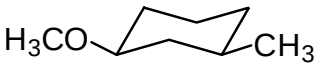
least stable most stable

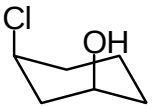
(a) 

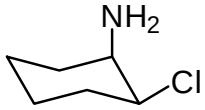
(b) 

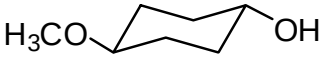
(c) 

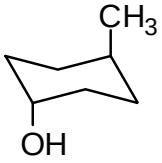
(d) 

(e) 

(f) 

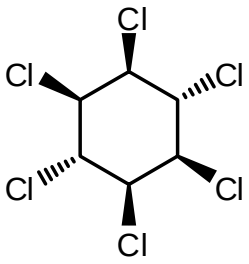
(g) 

(h) 

(h) 

(Hint: take a minute and draw in the corresponding axial or equatorial C-H bonds on the carbons where the groups are shown)

18. In each of these two molecules, how many of the Cl groups are equatorial when the molecule is in its most stable chair form? Draw the two chair representations of each.

(a) 

(b)