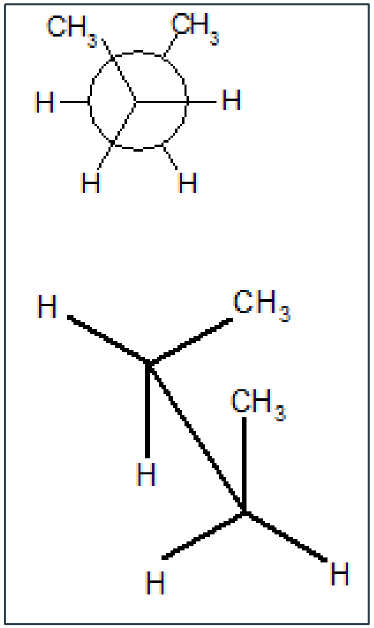
Organic Chemistry Chapter 6: Conformations

Alkanes, Chairs, and Newman Projections

Adapted from David Klein's Organic Chemistry as a Second Language

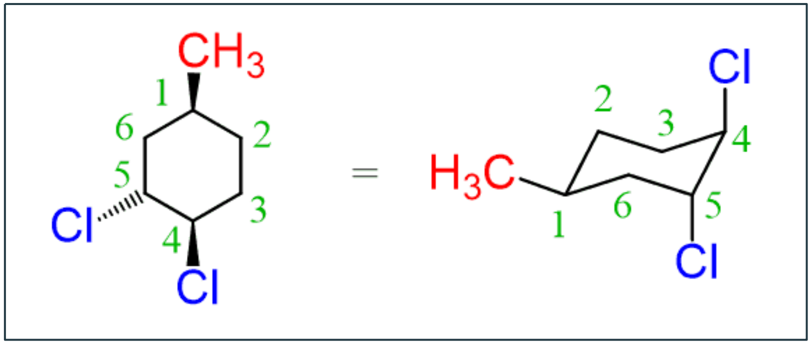
Chapter 6 Objectives:



Students will be able to:

1. Describe the need for conformation analysis as it relates to alkanes.
2. Draw Newman Projections for various alkanes.
3. Rotate and assess stability of Newman Projections.

4. Draw chair conformations of cyclohexanes, including all axial and equatorial positions.
5. Flip and assess the stability of various chair conformations.



Chapter 6 - Part 0

Real-World Applications of Alkanes

6.0 Relative Stability of Isomers

- To rationalize and predict the outcomes of chemical reactions, it is helpful to assess stability of compounds
- Remember: **stable** = **low** potential energy = **low reactivity** = **little energy** will be released upon reacting
- If you drove a car today, what type of chemical reaction with alkanes did you perform?

- What is the general reaction equation for the combustion of octane?

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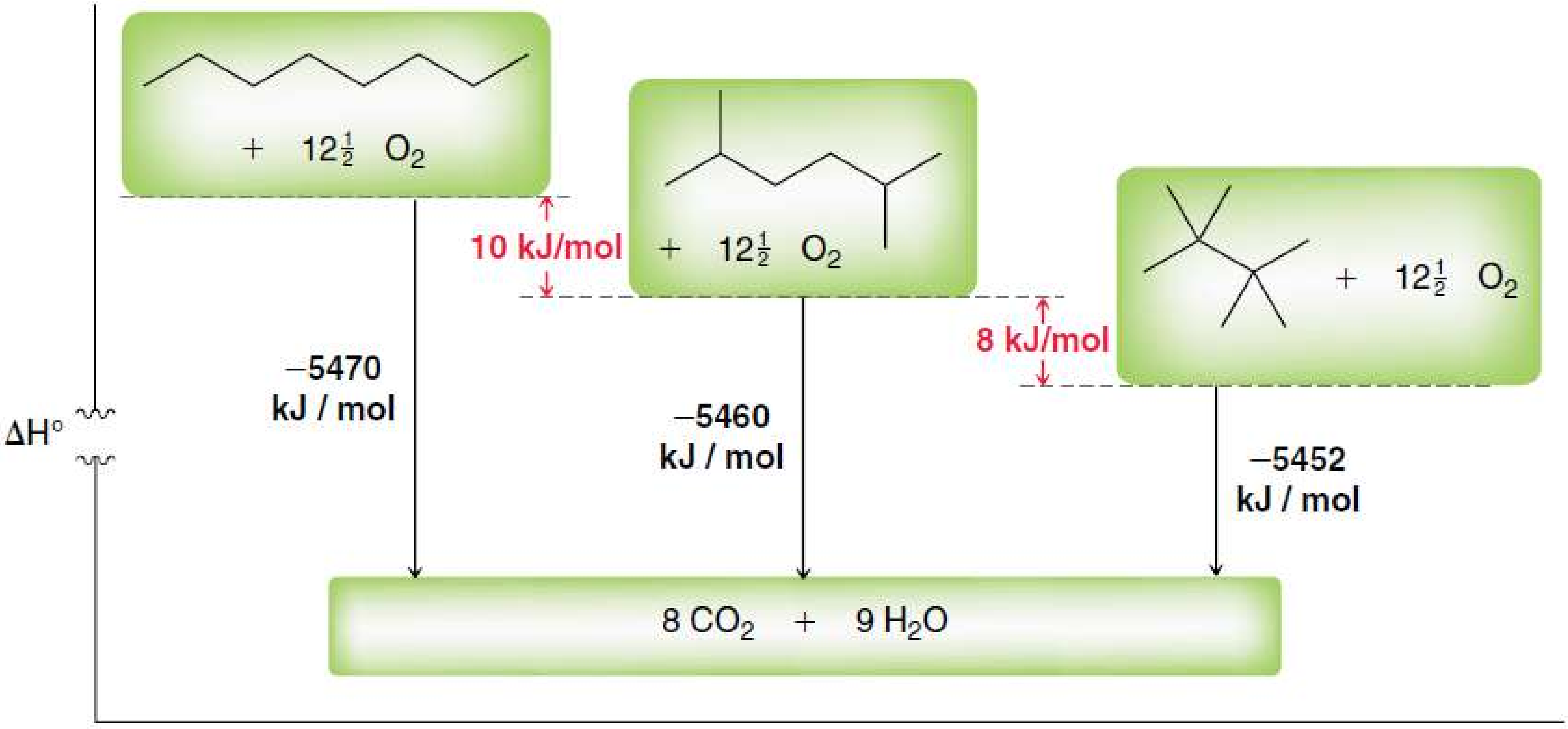
6.0 Relative Stability of Isomers

- Compare the heats of combustion for 3 octane isomers



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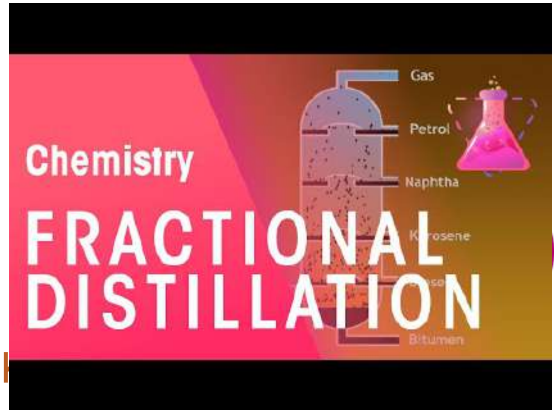
6.0 Sources and Uses of Alkanes

- Petroleum, which literally means rock oil is the main source of alkanes
- Petroleum is a mixture of hundreds of hydrocarbons, mostly alkanes with varying numbers of carbons and varying degrees of branching
- The alkanes in petroleum with 5 to 12 carbons per molecule are most valuable, and they can be separated from the rest of the oil by distillation
- HOW does distillation work?



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6.0 Sources and Uses of Alkanes

- Table 4.5 shows the various components of petroleum

TABLE 4.5 INDUSTRIAL USES OF PETROLEUM FRACTIONS

BOILING RANGE OF FRACTION (° C)	NUMBER OF CARBON ATOMS IN MOLECULES	USE
Below 20	$C_1 - C_4$	Natural gas, petrochemicals, plastics
20 – 100	$C_5 - C_7$	Solvents
40 – 200	$C_5 - C_{12}$	Gasoline
175 – 300	$C_{12} - C_{18}$	Kerosene, jet fuel
275 – 400	C_{12} and higher	Heating oil, diesel
Nonvolatile liquids	C_{20} and higher	Lubricating oil, grease
Nonvolatile solids	C_{20} and higher	Wax, asphalt, tar

- The gasoline fraction of crude oil only makes up about 19%

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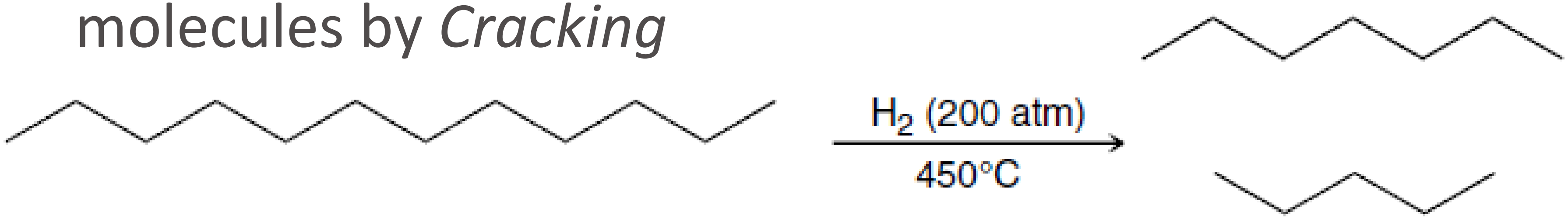
6.0 Sources and Uses of Alkanes

- Gasoline is a mixture of straight, branched, and aromatic hydrocarbons (5-12 carbons in size)
- Large alkanes can be broken down into smaller molecules by *Cracking*



- Straight chain alkanes can be converted into branched alkanes and aromatic compounds through *Reforming*
- After using these processes, the yield of gasoline is about 47% rather than 19%

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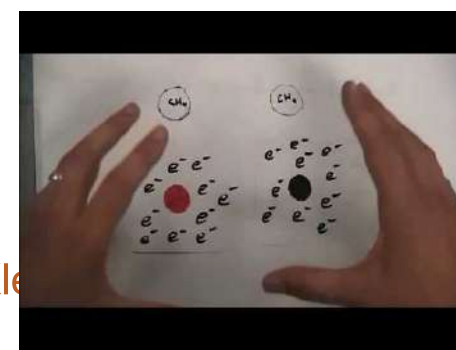
6.0 Sources and Uses of Alkanes

- At room temperature
  - Small alkanes with 1-4 carbons are gasses
  - Medium size alkanes with 5-12 carbons are liquids
  - Large alkanes with 13-20 carbons are oils
  - Extra large alkanes with 20-100 carbons are solids like tar and wax
  - Super-sized alkanes called polymers can have thousands or millions of carbon atoms in each molecule
- What type of properties would you expect such polymers to possess?
- Why? Consider London forces



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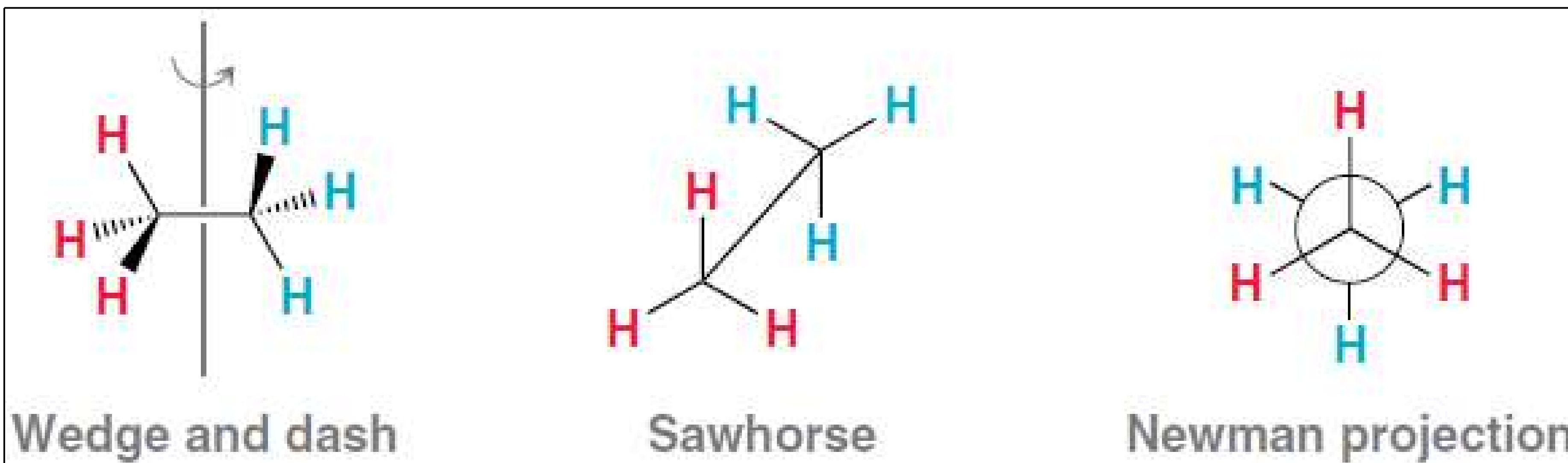
Chapter 6 - Part I

Newman Projections

Intro Crash Course Organic Chemistry Video for cycloalkanes. This provides a great overview of the entire chapter. We will first learn about Newman Projections, then about Chair Conformations.

6.1 Newman Projections

- We know that single bonds in molecules can rotate
- Different rotational states are called **conformations**
- 3D Rotational conformations are difficult to represent on a 2D paper. *It's useful to make a molecular model to help you visualize the structures*
- Here are three ways to represent ethane

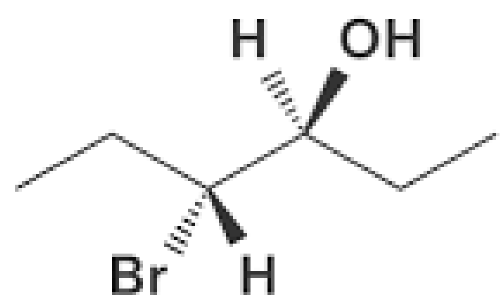


Review with Wedges and Dashes

1. It doesn't matter if the wedge is on the left or right

1. EACH tetrahedral carbon will have:
   - 2 straight bonds (in-plane of paper)
   - 1 wedge (coming towards you)
   - 1 dash (going away from you)

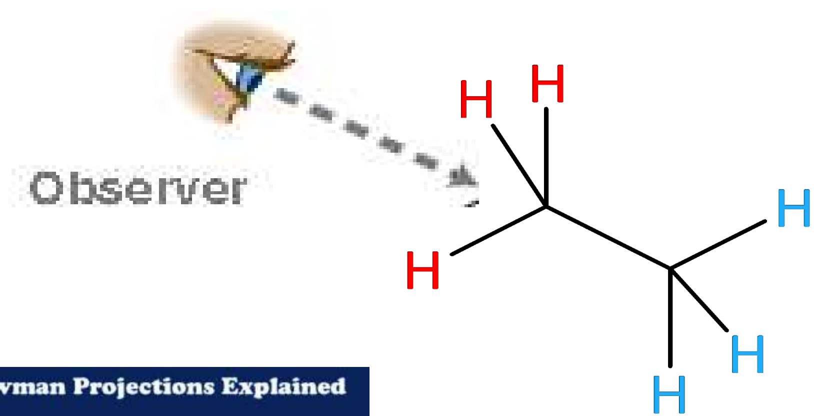
1. Sometimes we won't show all of the wedges/dashes, especially if they are H's attached to carbons

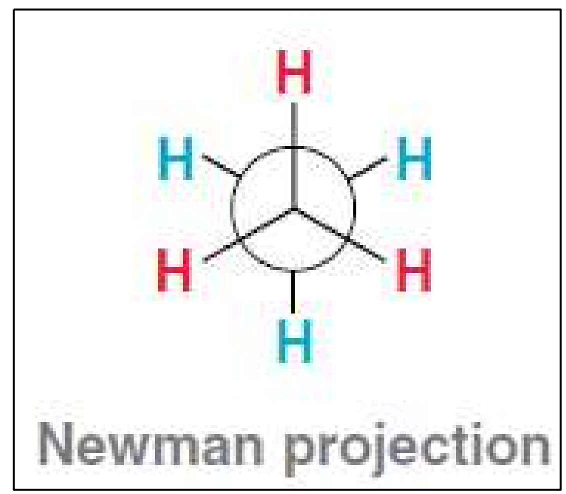


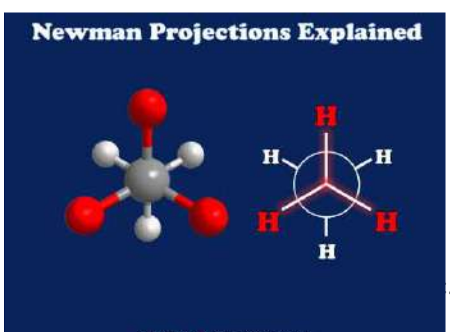
Wedge and dash

6.1 Newman Projections

- Look directly down the C-C single bond axis. This is where it is especially helpful to have a model
- The front carbon should eclipse the single bond and the carbon behind it
- Show the front carbon as a point and the back carbon as a large circle behind it



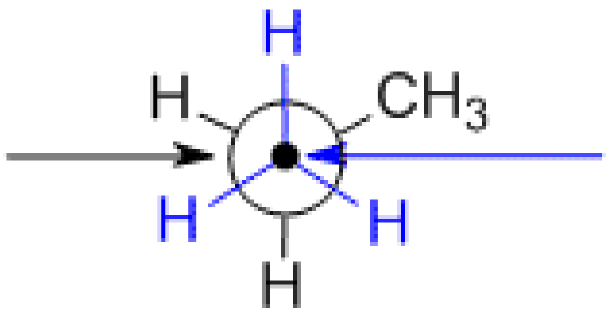




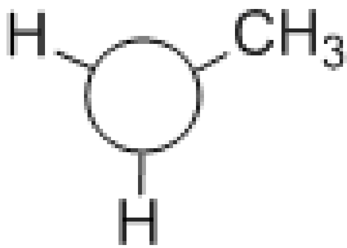
Introduction Video for Newman Projections

6.1 How to Draw Newman Projections

The "circle" defines the **back** carbon atom and the groups attached to it

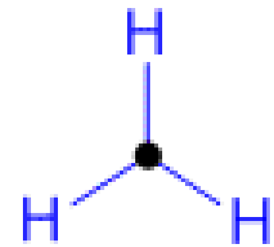


The "dot" defines the **front** carbon atom and the groups attached to it



back carbon only

Build these models with your kit!

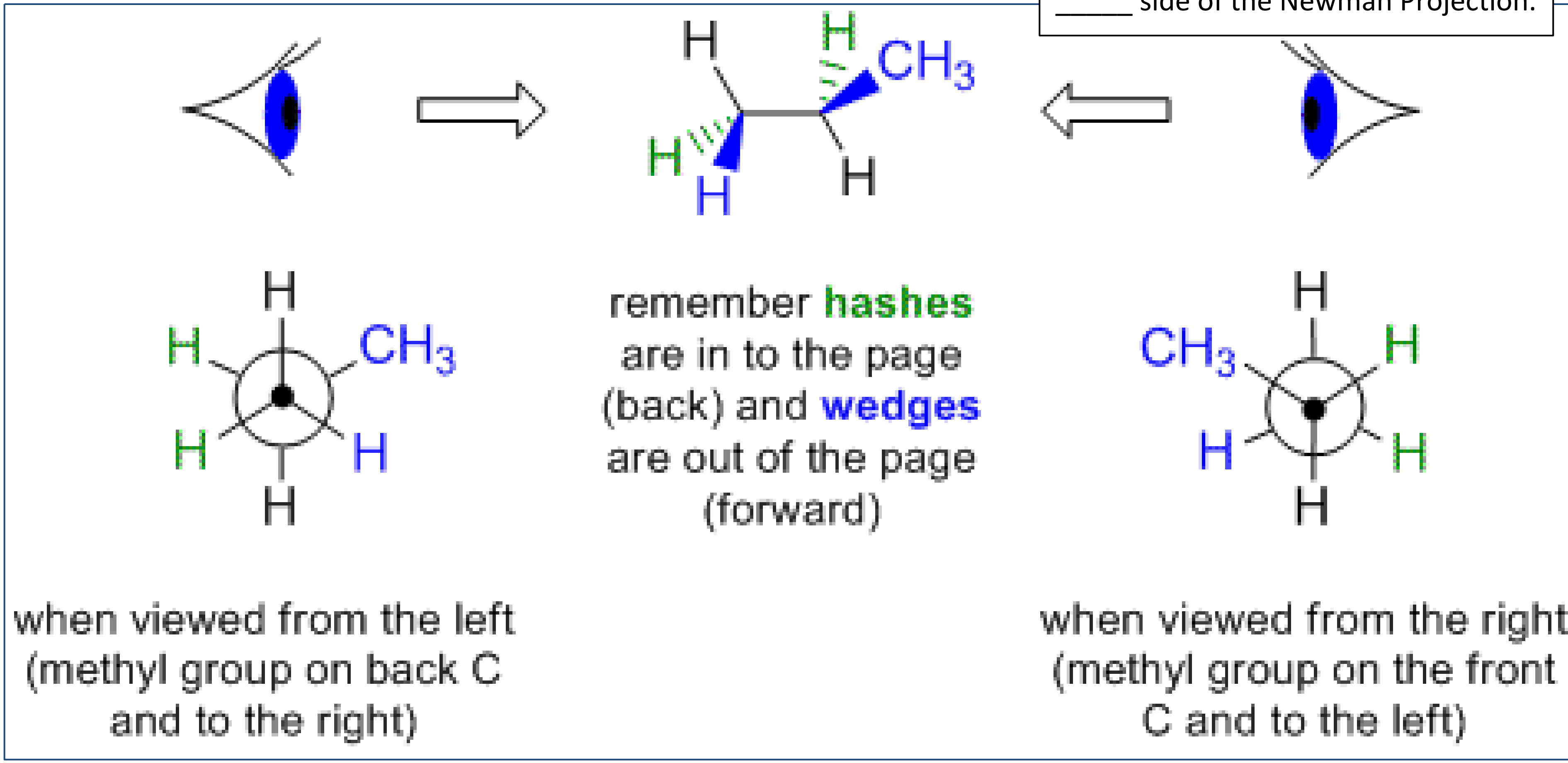


front carbon only

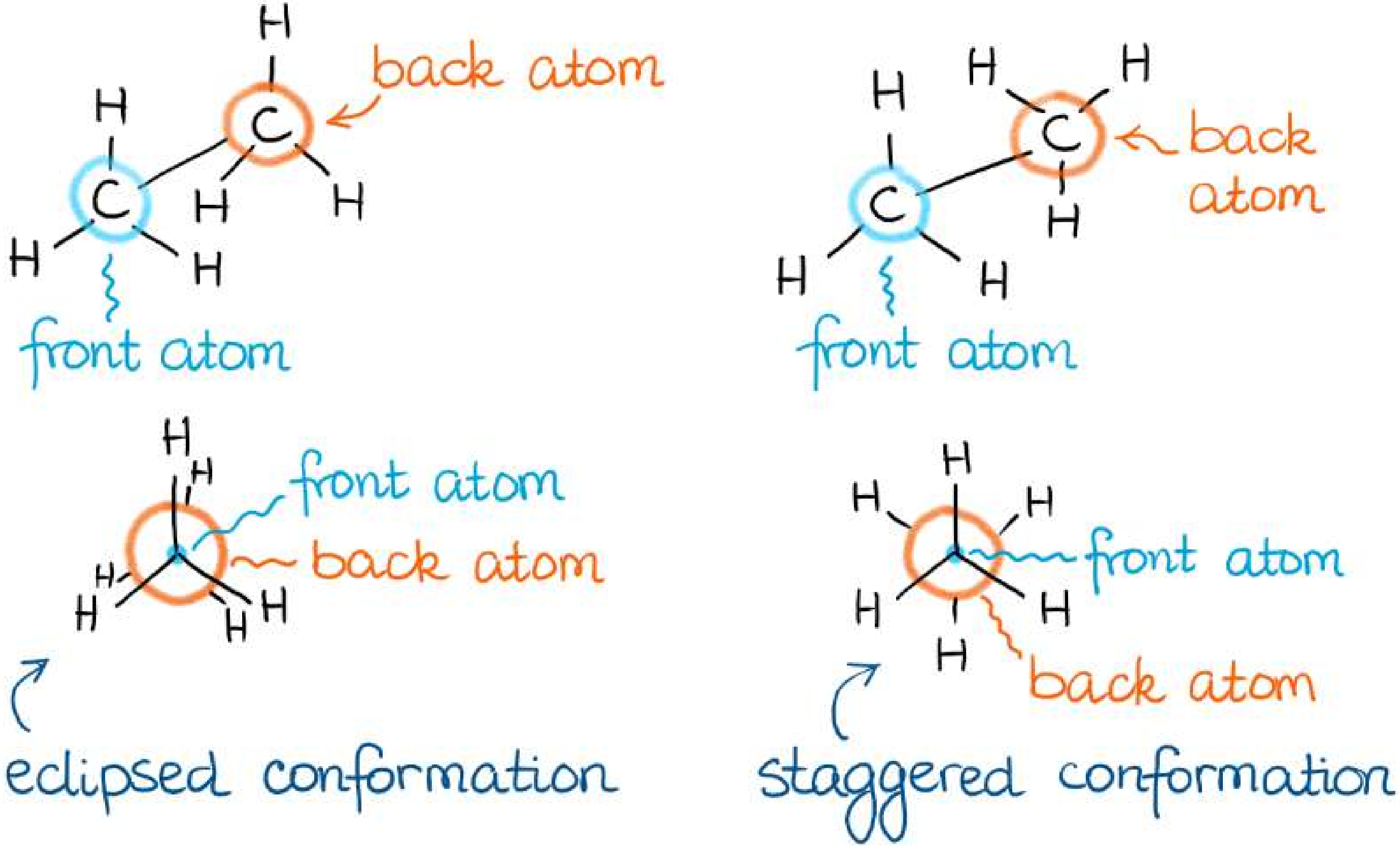
Newman

Newman Projections are all about PERSPECTIVE!

The methyl would be on the top
______ side of the Newman Projection.



There will usually be an arrow or eyes telling you which way to view your molecule from.



Short-Cuts we may see…

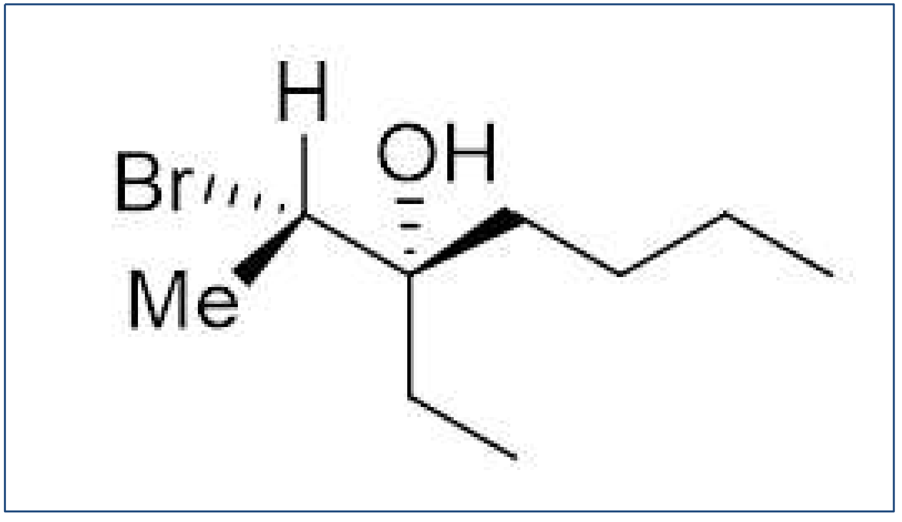
CH_3 = methyl = Me

CH_2CH_3 = ethyl = Et

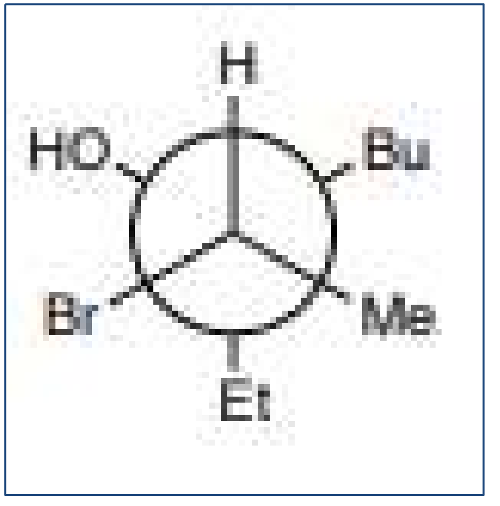
$CH_2CH_2CH_3$ = propyl = Prop

$CH_2CH_2CH_2CH_3$ = butyl = Bu or But

**There are many more - just try to reason them out!*

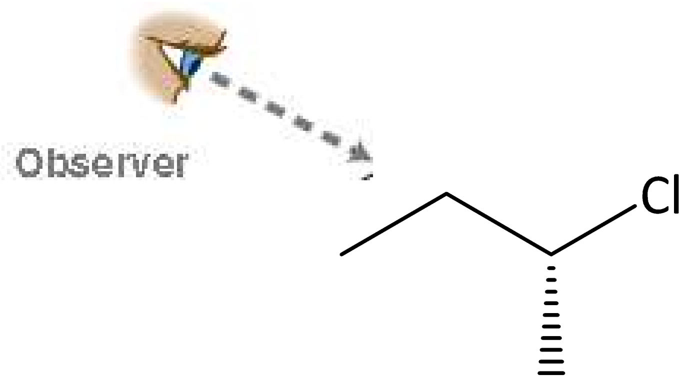


This wedge/dash drawing is the same as the Newman Projection



6.1 Newman Projections

- Draw a Newman projection for the following molecule



- How would it look if the observer were viewing it from the opposite direction?

READ Pages 106-110 in the Klein Packet, then complete problems 6.2-6.7

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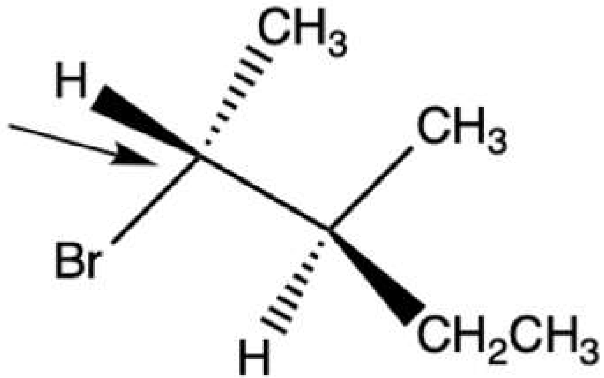
Let's Practice! Draw the Newman projection as it is shown (don't rotate yet!)

1. 

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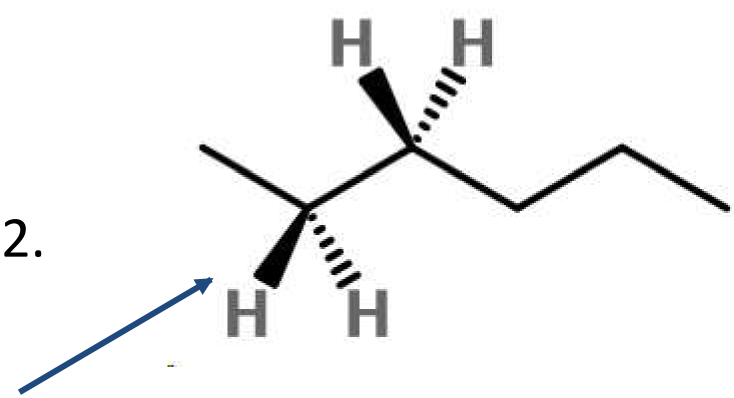
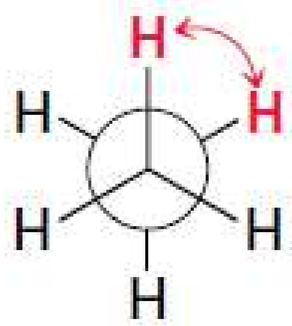
2. 

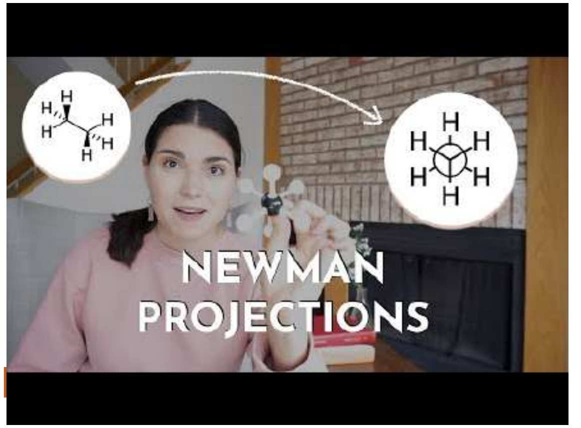
6.2 Rotational Conformations

- What is the angle between H atoms on the same carbon? In the Newman projection it looks like 120°.
- Does the angle affect stability? WHY? Think about areas of *high electron density repelling*
- The angle between H atoms on adjacent carbons is called a dihedral or **torsional** angle. It is 60° in the molecule below



Dihedral angle = 60°

2 Strategies and Practice with Newman Projections Video



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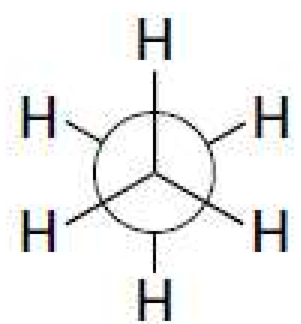
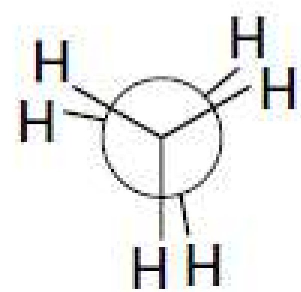
6.2 Rotational Conformations

- If ethane were to rotate 60° about the C-C bond, the the H atoms on adjacent carbons eclipse one another
- Compare the stability of the **eclipsed** and **staggered** conformations based on the repulsion of areas of high electron density



Staggered conformation
Lowest in energy



Eclipsed conformation
Highest in energy

- What other conformations are possible?

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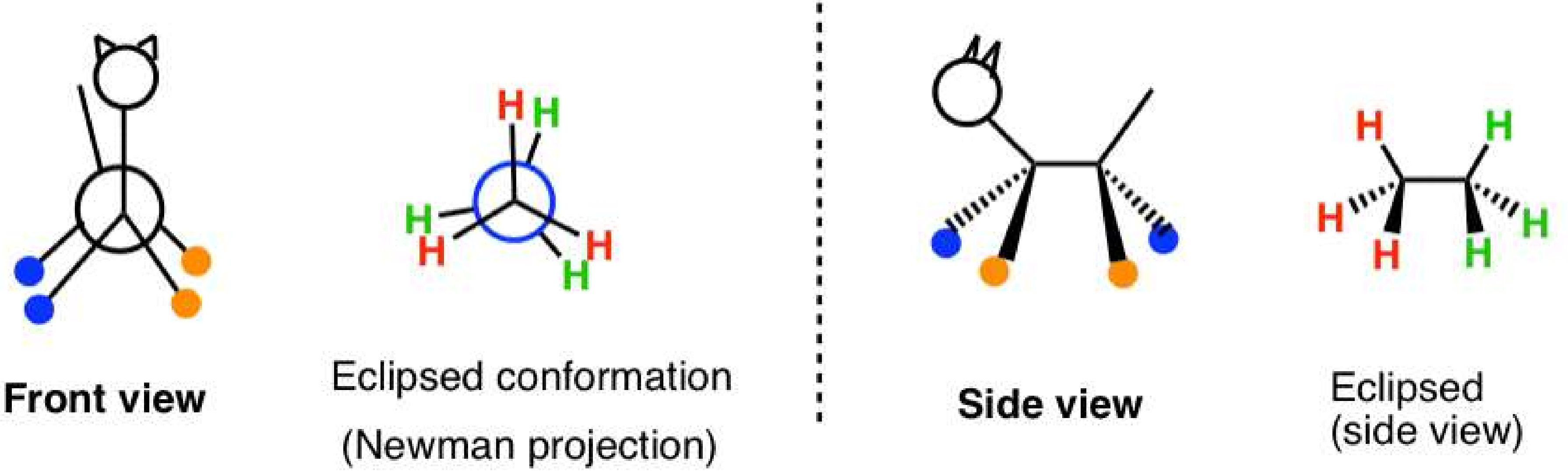
Sometimes the molecules given have an “eclipsed” formation



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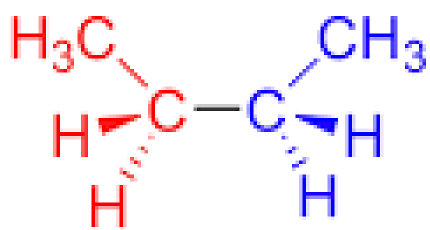

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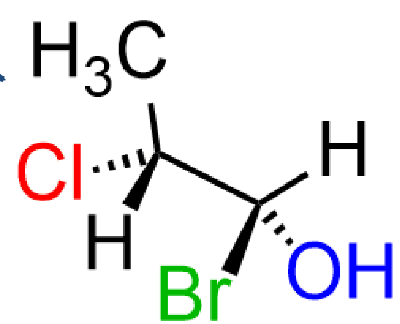
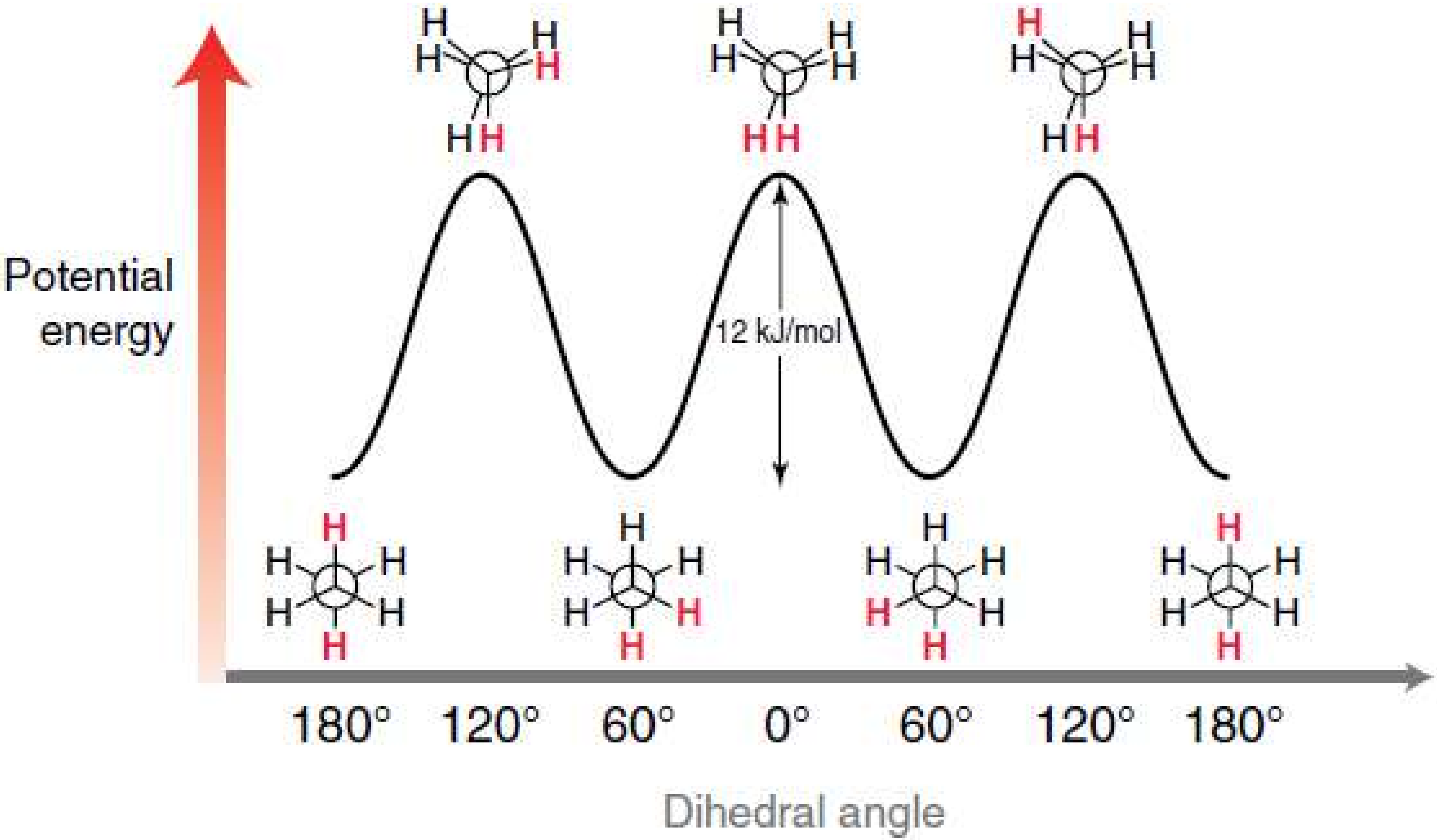


6.2 Rotational Conformations

- Consider a complete 360° rotation about the C-C bond



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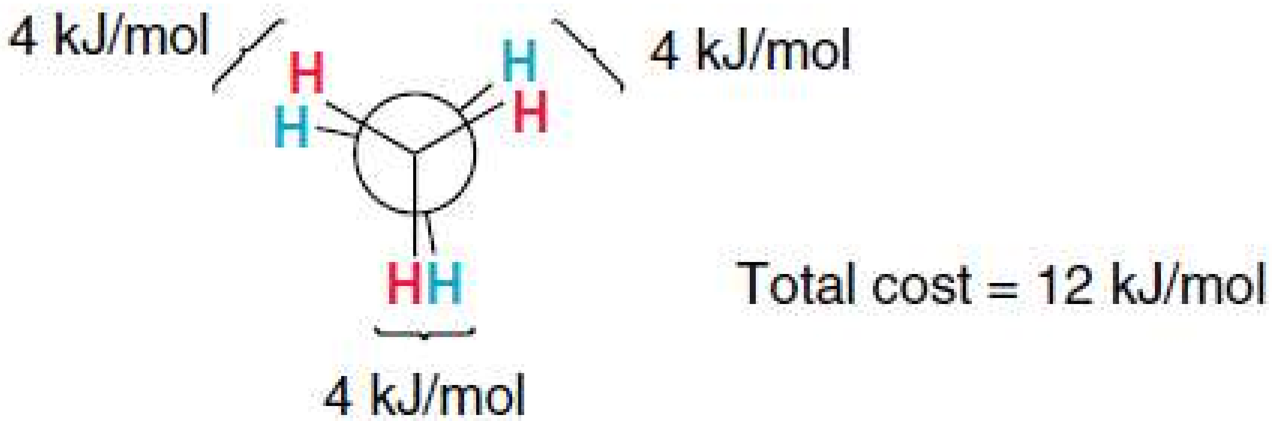
6.2 Rotational Conformations

- The difference in energy between the staggered and eclipsed conformations is called **torsional strain**
- *With a difference of 12 kJ/mol in stability, at room temperature, 99% of the molecules will be in the staggered conformation*



- How would the ratio change at a higher temperature?

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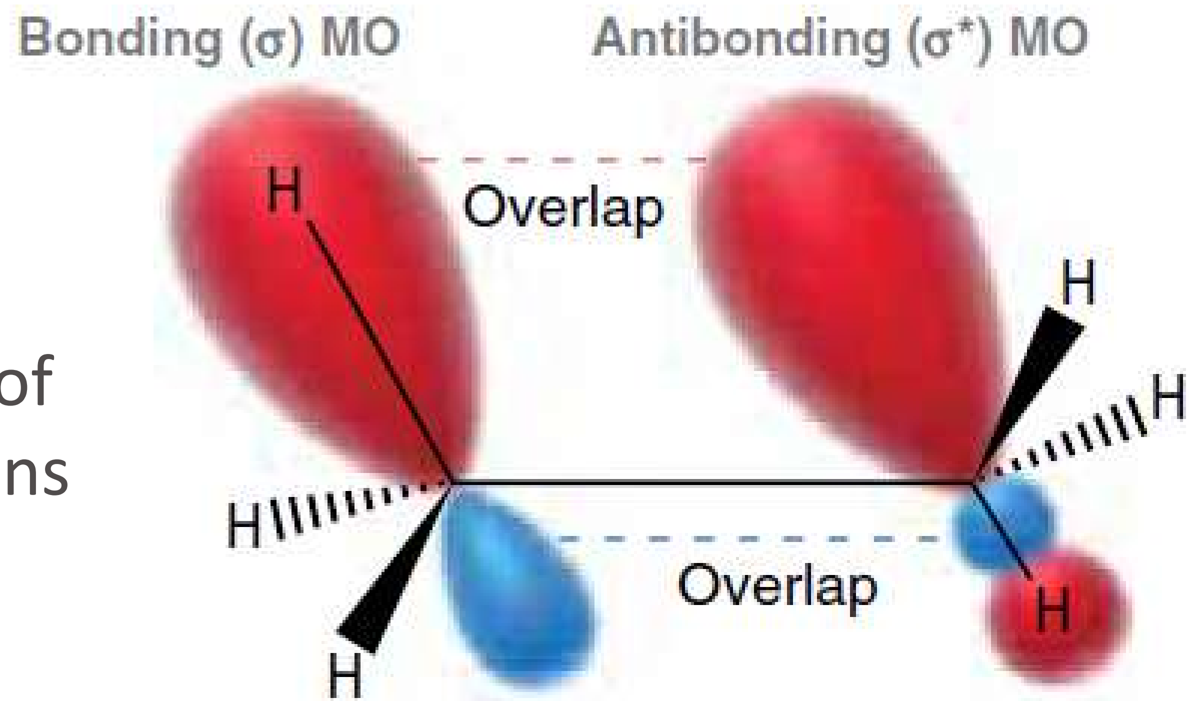
6.2 Rotational Conformations

- **Torsional strain** can also be explained using molecular orbital theory

- In the staggered conformation, the bonding and antibonding MOs of neighboring carbons overlap



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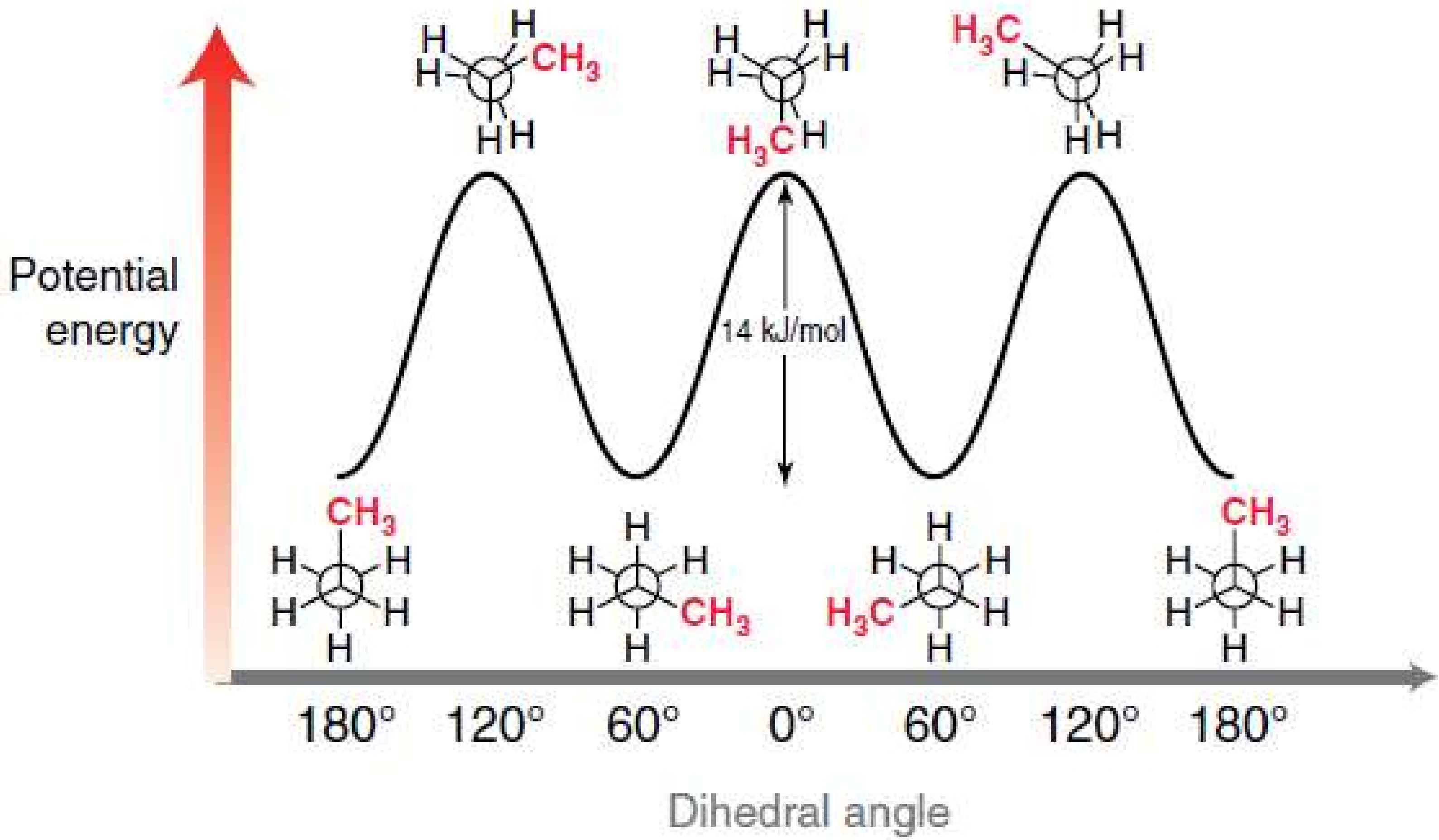
6.2 Rotational Conformations

- The analysis of **torsional strain** for propane shows a very similar situation



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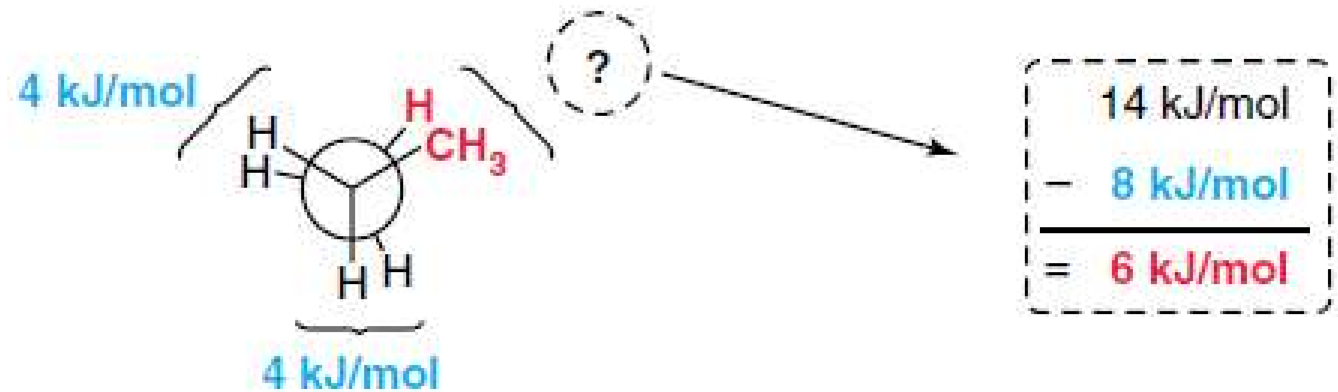
6.2 Rotational Conformations

- The **torsional strain** for propane is 14 kJ/mol, which is 2 kJ/mol more than for ethane
- If each H-----H eclipsing interaction costs 4 kJ/mol of stability, that total can be subtracted from the total 14 kJ/mol to calculate the contribution of a CH_3-----H eclipsing interaction



- Practice with conceptual checkpoint 4.19

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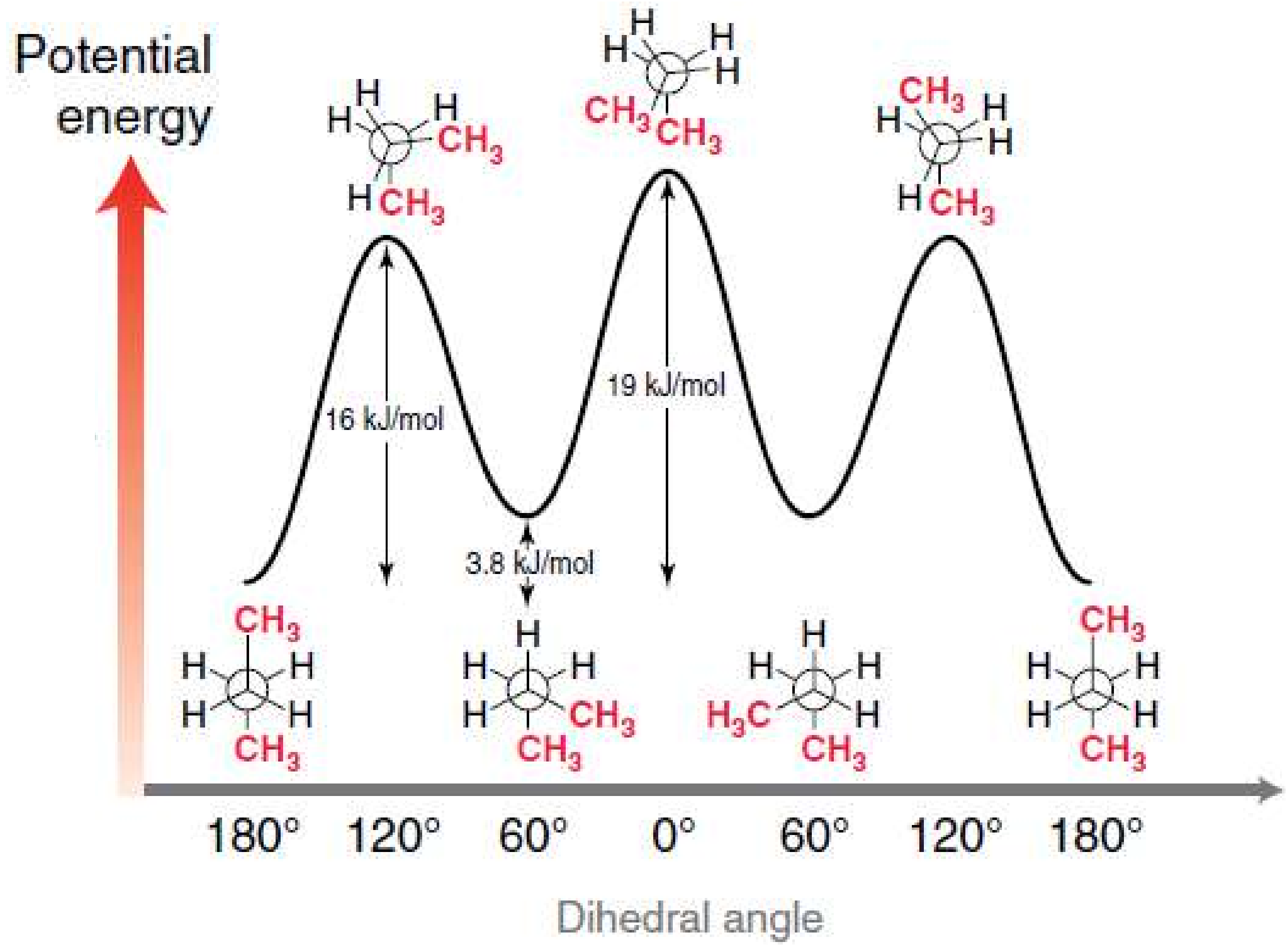
6.2 Butane's Conformations

- The analysis of **torsional strain** for butane shows more variation

- Note that there are multiple staggered conformations and multiple eclipsed conformations



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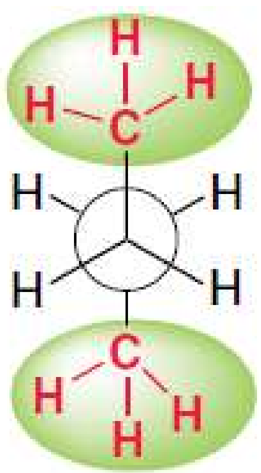
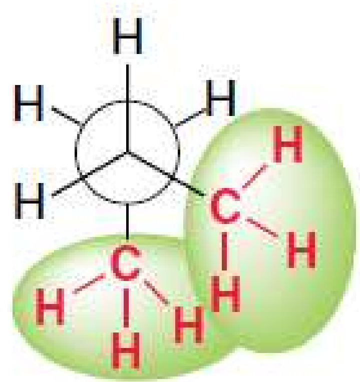
6.2 Butane's Conformations

- The stability of the different staggered conformations differs by 3.8 kJ/mol
- The anti conformation has less steric hindrance.



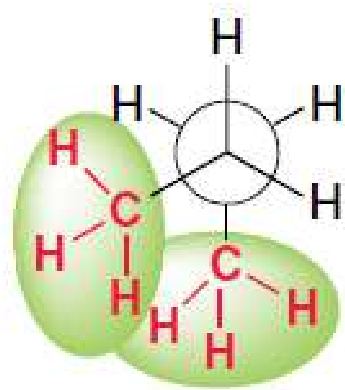
Anti

Methyl groups are farthest apart



Gauche

Methyl groups experience a gauche interaction



Gauche

Methyl groups experience a gauche interaction

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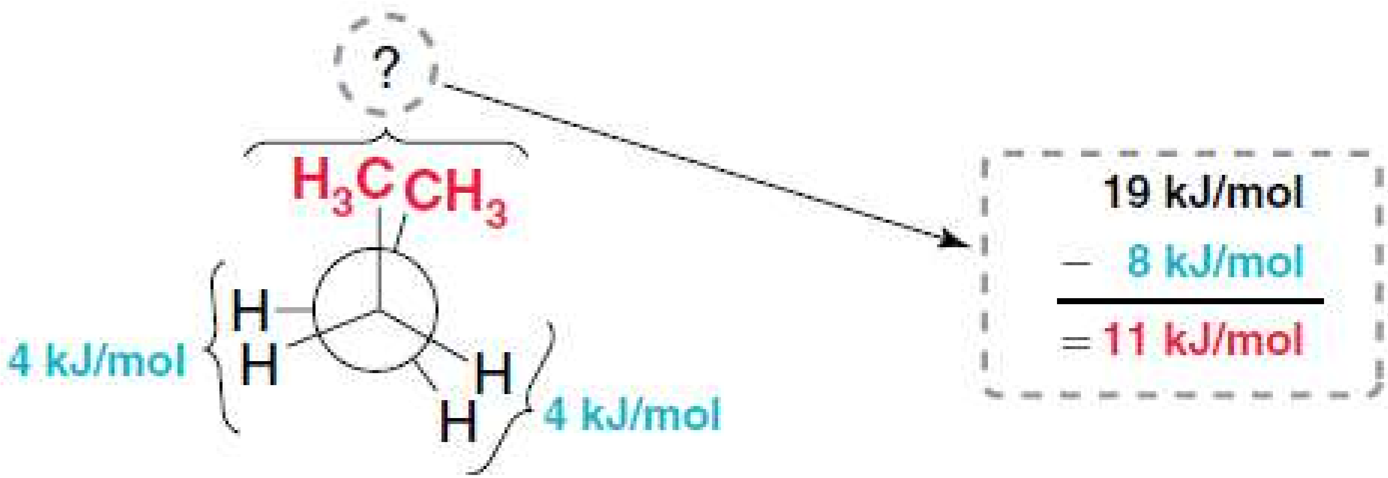
6.2 Butane's Conformations

- The least stable conformation results when the methyl groups eclipse one another



- Each CH_3-----CH_3 **eclipsing** interaction accounts for 11 kJ/mol of energy (torsional and steric strain).

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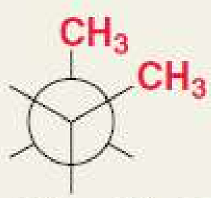
6.2 Butane's Conformations

- The values in table 4.6 can be used to predict relative energies for various conformations

*We don't have to do this for regular points in HS!

INTERACTION	TYPE OF STRAIN	ENERGY COST (KJ/MOL)
 H—H Eclipsed	Torsional strain	4
 CH_3—H Eclipsed	Torsional strain	6
 CH_3—CH_3 Eclipsed	Torsional strain + steric hindrance	11
 CH_3—CH_3 Gauche	Steric hindrance	3.8

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6.2 Rotational Conformations

- Draw a Newman projection for the highest and lowest energy conformations for 2,2,3,5,5-pentamethylhexane from C3 to C4. *(you will have to rotate the bonds)*

READ Pages 112-113 in the Klein Packet, then complete problems 6.9-6.14

Recap the Stability of Newman Projections

Staggered		Eclipsed
Anti	Gauche	
Most Stable	**Stable**	**Least Stable**

Extra Practice

Draw Newman projections for each of the following situations.

1. The highest energy conformation of 3-methylnonane along the C4 to C5 bond axis

1. The lowest energy conformation of trans-1-bromo-2-methylhexane along the C1 to C2 axis

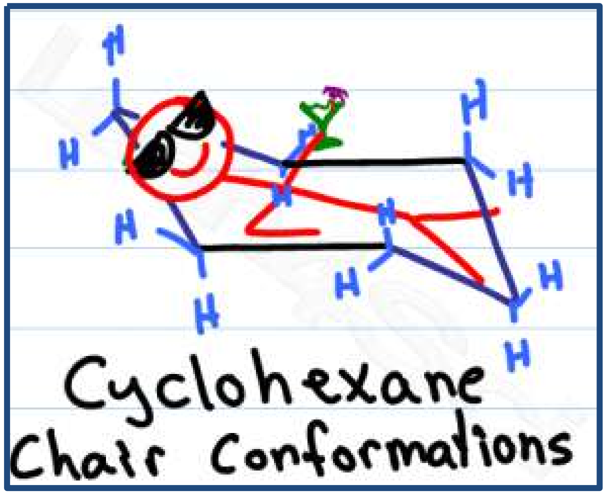
Practice Drawing Newman Projections from Names

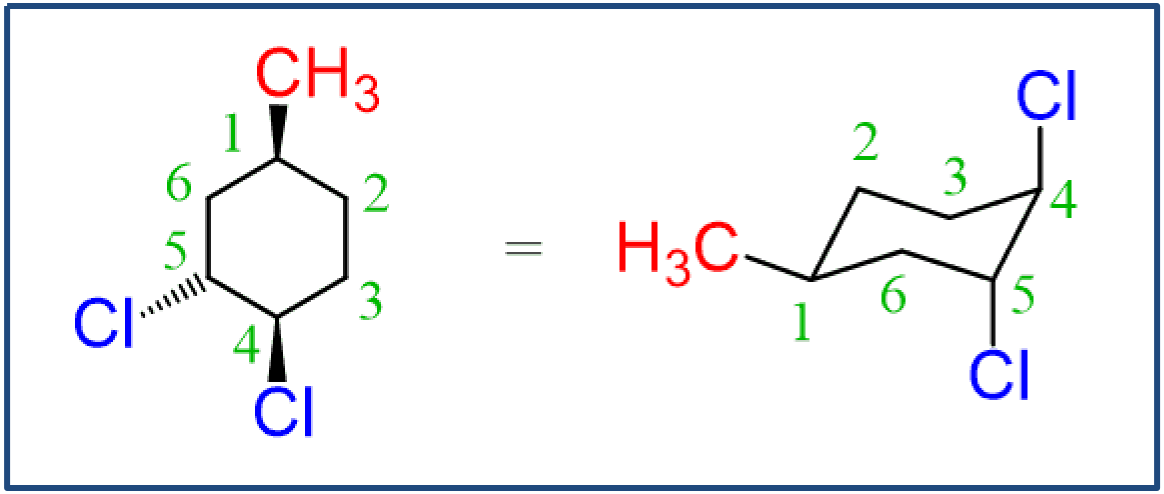
3. The lowest energy conformation of 7-ethyl-2,3,8-trimethyldecane along the C-5 to C-6 bond axis

Name: ______________________________

Chapter 6 - Part II

Chair Conformations

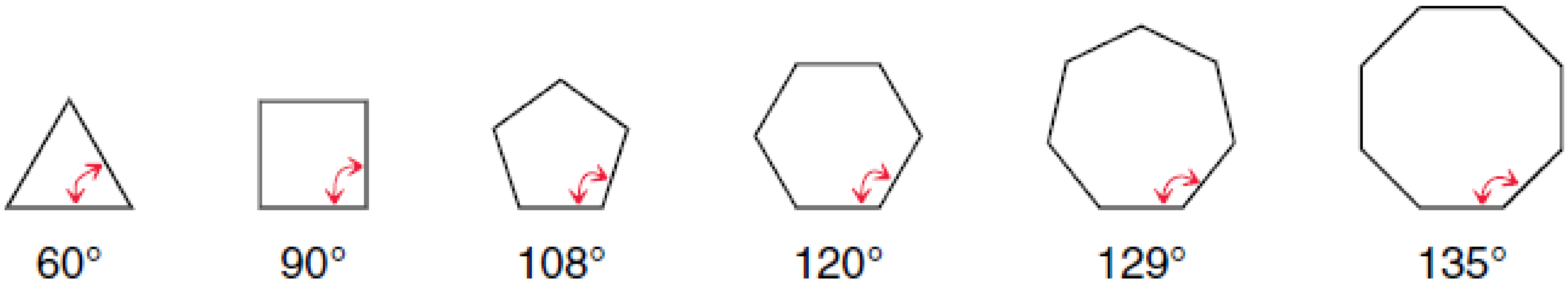




Intro Crash Course Organic Chemistry Video for cycloalkanes

6.3 Cyclic Alkanes

- Carbon atoms in alkanes are sp^3 hybridized
- What bond angles are optimal for such carbons?
- **If cycloalkanes were flat**, what bond angles would be expected?



- To optimize the bond angles, most cycloalkanes are NOT flat in their most stable conformation
- **Build a cyclohexane without the hydrogens**

6.3 Cyclic Alkanes

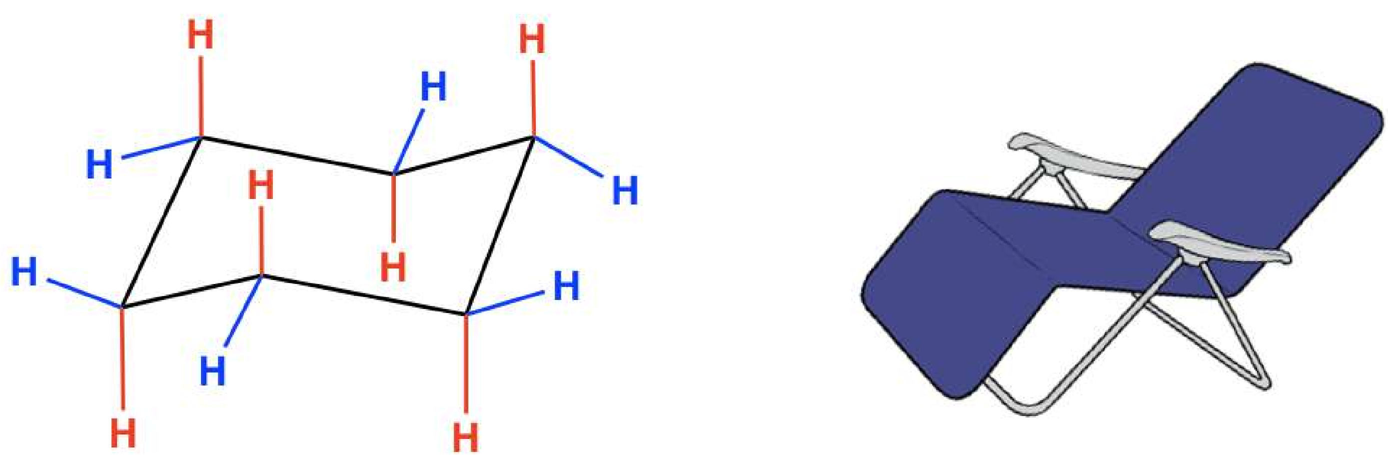
- Why are heats of combustion reported per CH_2 group?
- Considering the data in the table which ring has the least **ring strain**?

CYCLOALKANE	NUMBER OF CH_2 GROUPS	HEAT OF COMBUSTION PER CH_2 GROUP (KJ / MOL)
Cyclopropane	3	697
Cyclobutane	4	680
Cyclopentane	5	658
Cyclohexane	6	653
Cycloheptane	7	657
Cyclooctane	8	658
Cyclononane	9	659
Cyclodecane	10	659
Cycloundecane	11	661
Cyclododecane	12	654

6.3 Cyclohexane

- Cyclohexane is considered to have ZERO ring strain in its optimal conformation, **THE CHAIR**
  1. No angle strain - angles must be 109.5°
  2. No torsional strain - all adjacent C-H bonds must be staggered

Axial Positions are vertical, **equatorial positions** go around the outside like the equator. (or a tutu!)

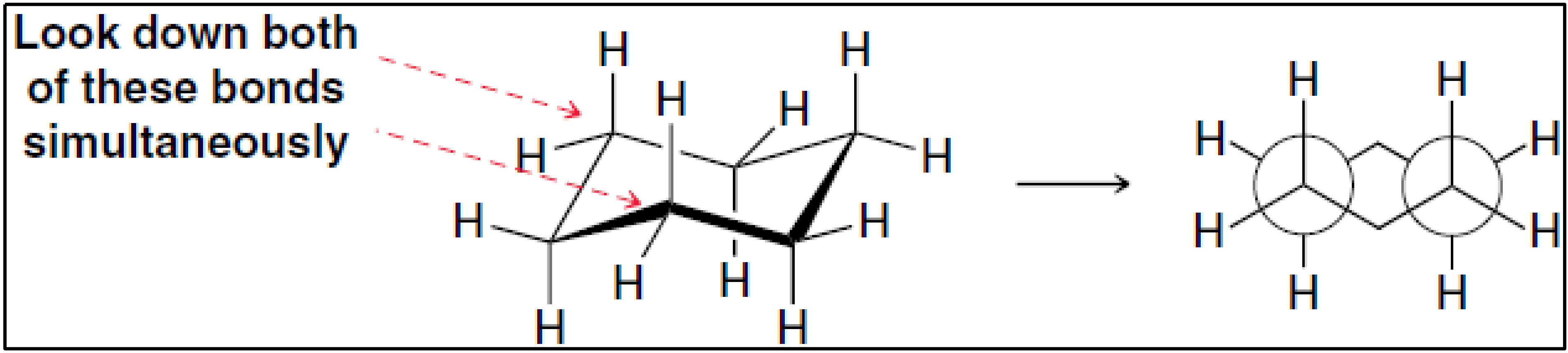


Chair conformation of cyclohexane

Chairs & Newman Projections

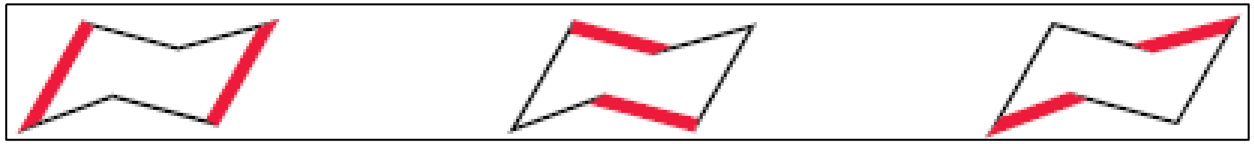
Chairs can be drawn like 2 Newman Projections, but we don't often to this in HS organic chemistry.

Add the H's on to your carbon cyclohexane to create the chair. Look down the planes like in the picture below.



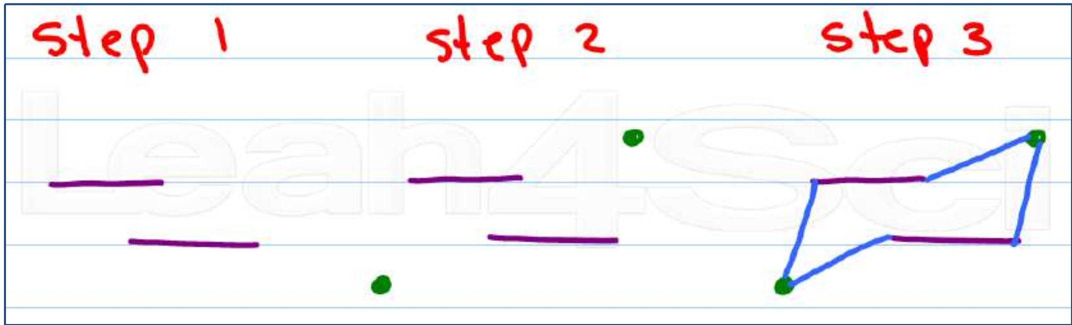
6.3 Drawing Chairs

- **It is critical to draw a CHAIR properly.** Use three sets of parallel lines



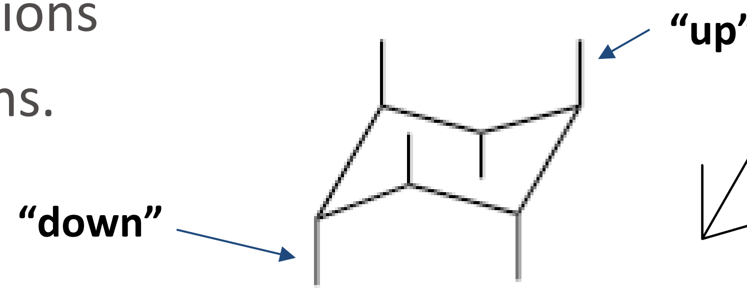
- Let's Practice in the space below! *Draw at least 6 chairs!*

You can also use this "hack" to draw your "forward" chairs!

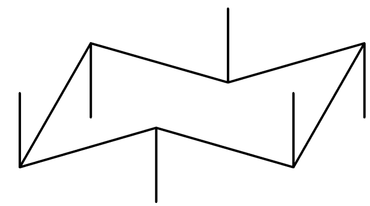


6.3 Drawing Axial Positions

- SIX of the atoms attached to the chair are **axial**. Axial groups point straight up and down alternating around the ring. *Mrs. H likes to start with what she calls "carbon #1" it is vertically "up".*
- Practice drawing 3 chairs with axial positions in the space below
  - there are 3 axial "up" positions
  - and 3 axial "down" positions.



Correct

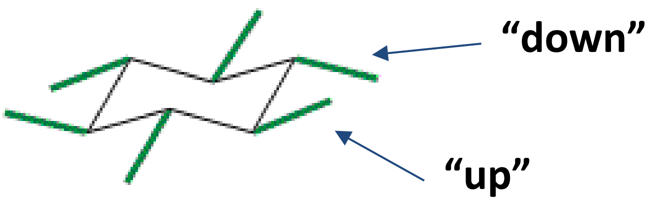


Incorrect

6.3 Drawing Equatorial Positions

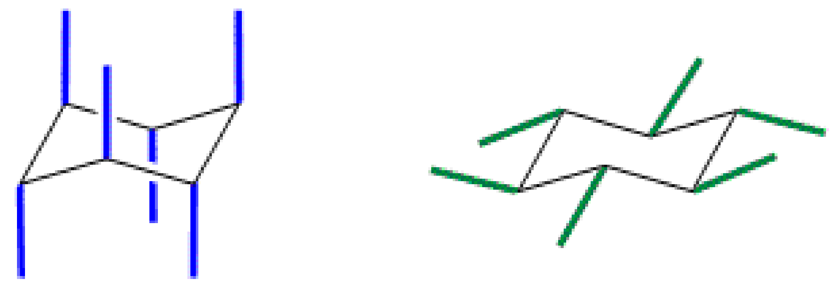
- SIX of the atoms attached to the chair are **equatorial**. Equatorial substituents are positioned at angles parallel to the sets of parallel lines making up the chair itself. *Mrs. H likes to start with what she calls "carbon #1" it is equatorial "down", it will alternate between "up" and "down" just like the axial positions.*

- Practice drawing 3 chairs with equatorial positions in the space below
  - there are 3 equatorial "up" positions
  - and 3 equatorial "down" positions.



6.3 Putting it all together

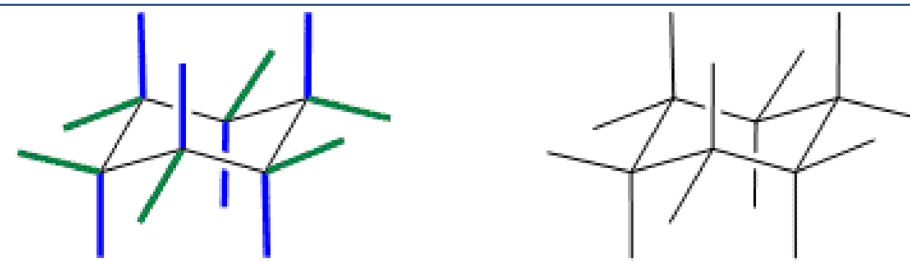
1. Start by drawing your chair shape, making sure to watch your parallel lines!
2. Then add all the axial positions, alternating “up, down, up, etc”
3. Then all the equatorial position, this time starting with “down, up, down etc.



axial positions

equatorial positions

Now it is your turn! Draw out 2 chairs with all the axial and equatorial positions labeled!

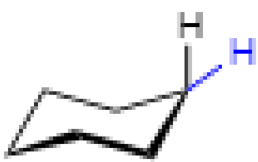


axial & equatorial positions

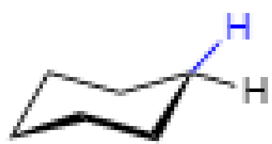
typical drawing showing all the axial and equatorial positions. Each C looks tetrahedral

6.3 Mistakes to Avoid

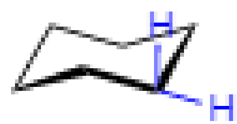
1. Make sure your outside lines are parallel.
2. Axial likes should be vertical!
3. Equatorial lines will be parallel with other lines in the structure of your chair.
4. EACH carbon will have an “up” and “down” position that alternates axial and equatorial



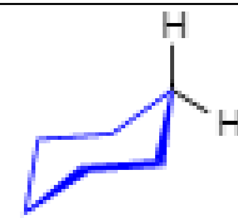
Incorrect.
Equatorial bond should be **down** and out.



Incorrect.
Axial bond should be **straight up.**

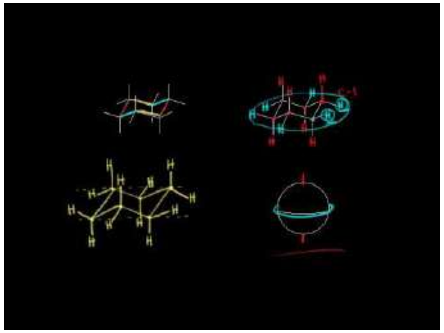


Incorrect.
Axial bond should be **straight down**, equatorial bond should be **up** and out.



Incorrect.
Ring should be tilted slightly.

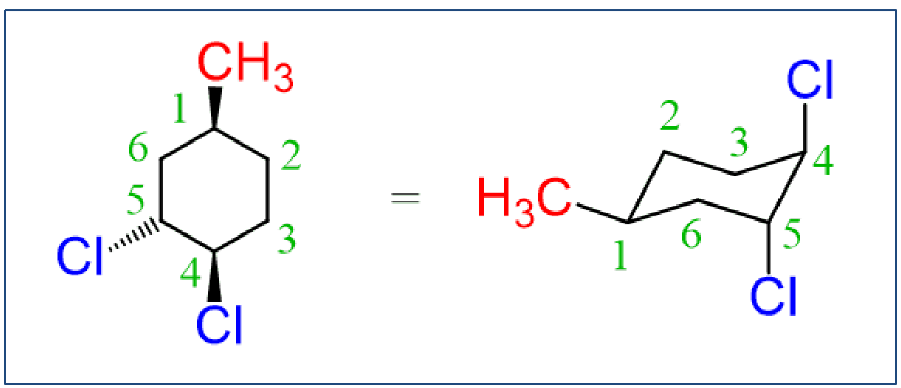
Video tutorial for drawing/labeling chairs. Note: It also shows the flipped chair towards the end!

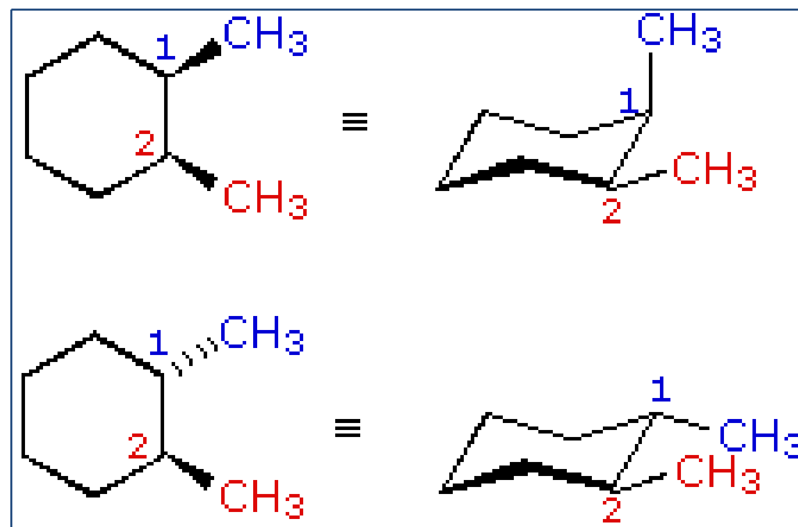


READ Pages 115-118 in the Klein Packet (Section 6.3)

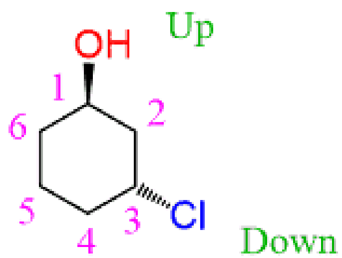
6.4 Placing Groups on the Chair

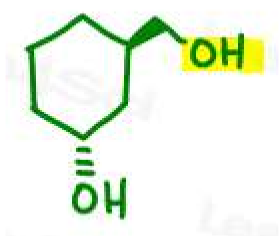
1. **Wedges** are coming towards us on the paper, these will be in an **"up"** position.
2. **Dashes** are going into the plane of the paper, these will be in a **"down"** position
3. *You can actually start at any carbon*, but Mrs. H. likes to always reference the top carbon on the cyclohexane an the top right on the ring as carbon #1 and move clockwise. *(They aren't the same numbers as we use in naming - we could rotate this around!)*
4. **You only need to show the axial & equatorial positions of the carbons that have "stuff" on them.**





6.4 Practice Making a Cyclohexane into a Chair

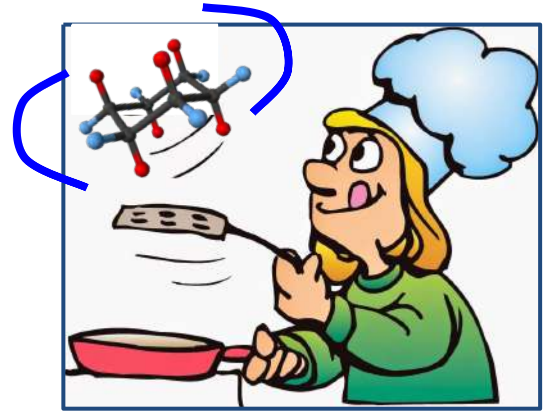




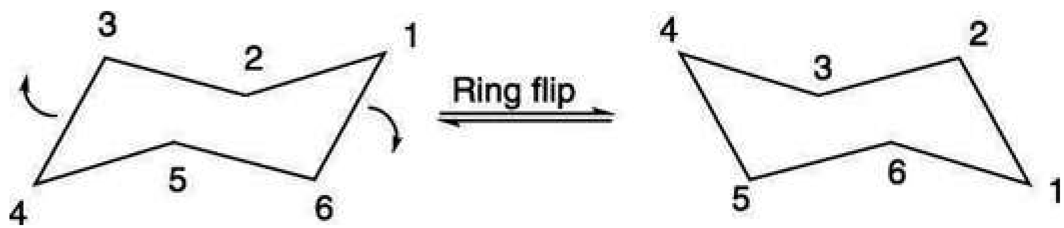
READ Pages 118-122 in the Klein Packet (Section 6.4) and complete **practice problems 6.15-6.21**

6.5 Ring Flipping

- Flipping a chair is not like flipping a pancake. Flipping a chair is the result of C-C single bonds rotating ONLY.



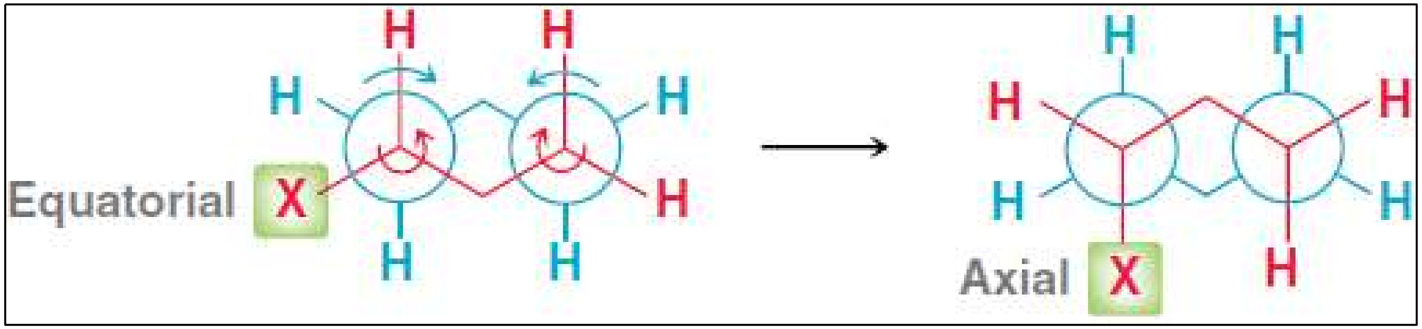
- It is actually more of a “shimmy” or “shift”
- Notice the slant or direction of the ring has shifted.



- Practice drawing 2 of the flipped (reversed) rings below!

6.5 More About Ring Flipping

- The Newman projection below shows how flipping occurs ONLY through rotating bonds and how it will affect the axial or equatorial position of the substituent

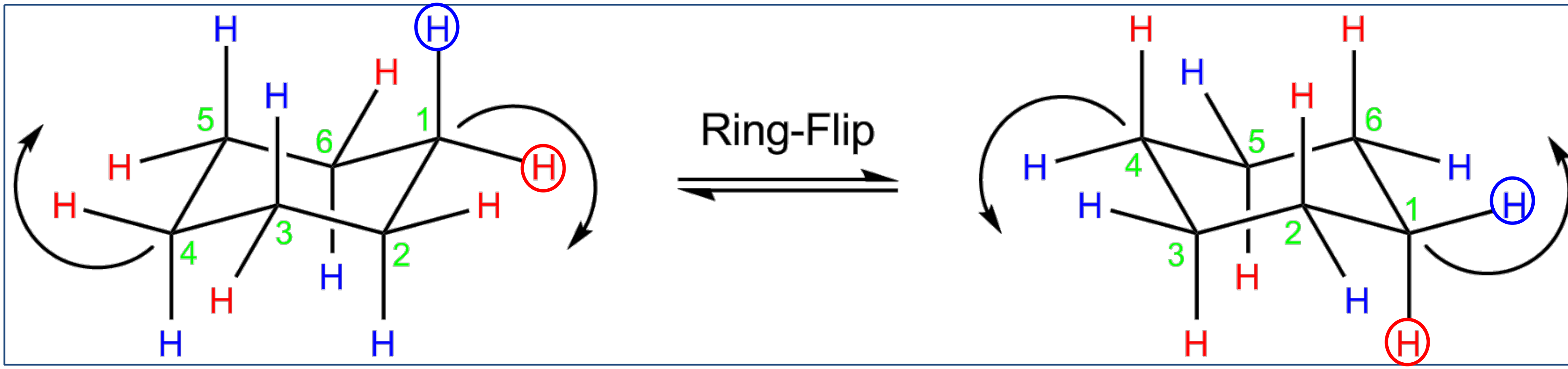


- Such flipping is MUCH easier to see with a handheld model. Try it yourself! *(Make the substituents alternating colors of white and green)*
- *What happens when you flip the ring to yo*

  positions?
- *What about the up/down aspect?)*

6.5 Ring Flipping

- We have to learn the equatorial and axial positions of the flipped chair as well.
- **Notice that only the concept of axial/equatorial is switching. the "up/down" terminology stays the same!**

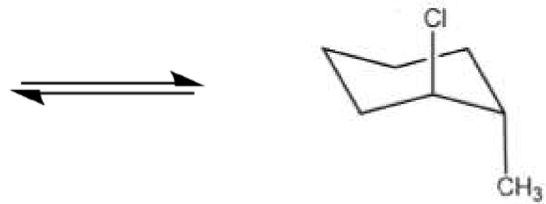


- *Practice drawing 2 of the flipped (reversed) rings below with all of the axial/equatorial positions drawn!*

6.5 Practice Doing a Ring Flip

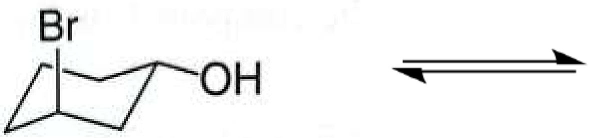
[CLICK HERE](#) for the answers!

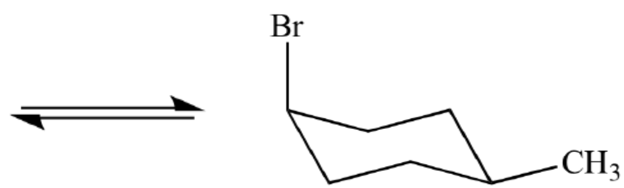
1.



Work backwards!

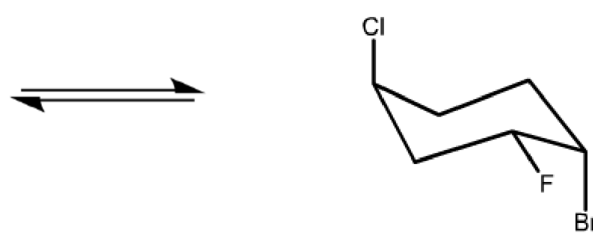
2.





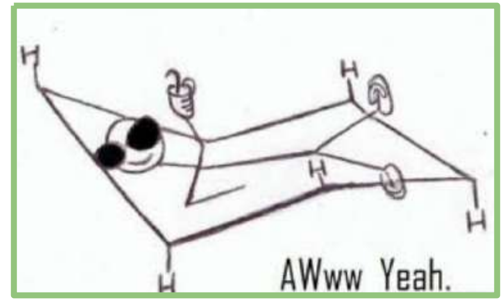
Work backwards!

3.

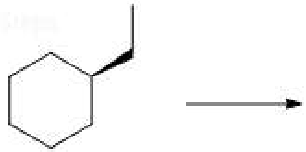


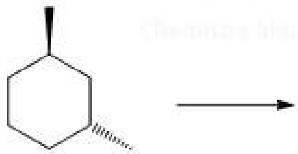
Work backwards!

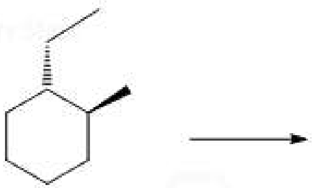
6.5 Practice Making Both Chairs

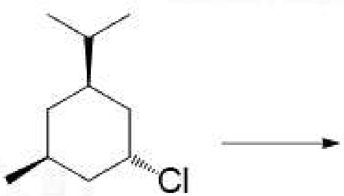


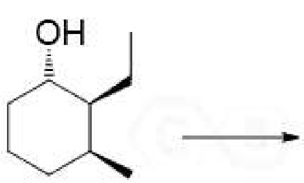
[CLICK HERE](#) for the answers!

a) 

b) 

c) 

d) 

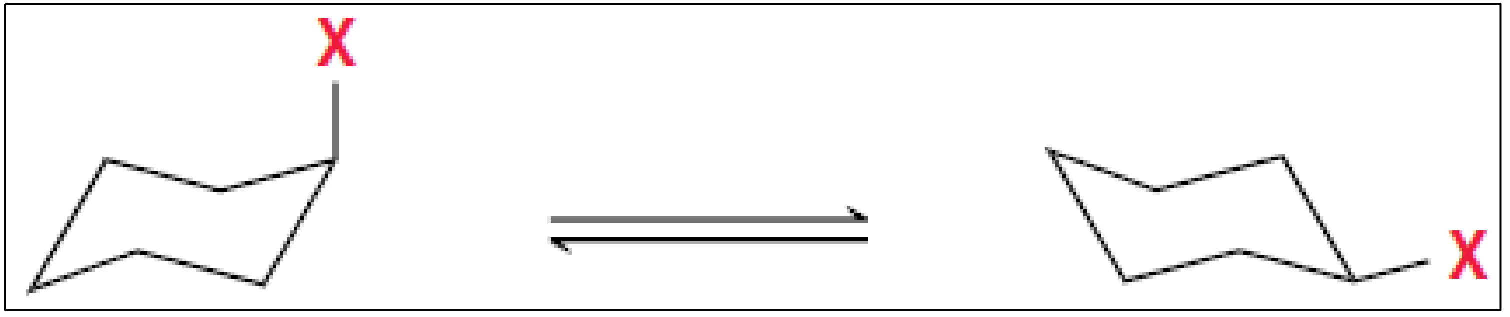
e) 

READ Pages 118-123 in the Klein Packet (Section 6.5) and complete **practice problems 6.22-6.36**

6.6 Comparing the Stability of Chairs

- The vast majority of cyclohexane molecules will exist in the chair conformation at any given moment. WHY?

- When energy (45 kJ/mol) is available, it can ***flip*** from one chair form to another.
  – Why do you think energy is needed? *(Think of spontaneous things in nature!)*
  – *Which "position" (axial or equatorial) do you think is more "comfortable" for the substituent?*



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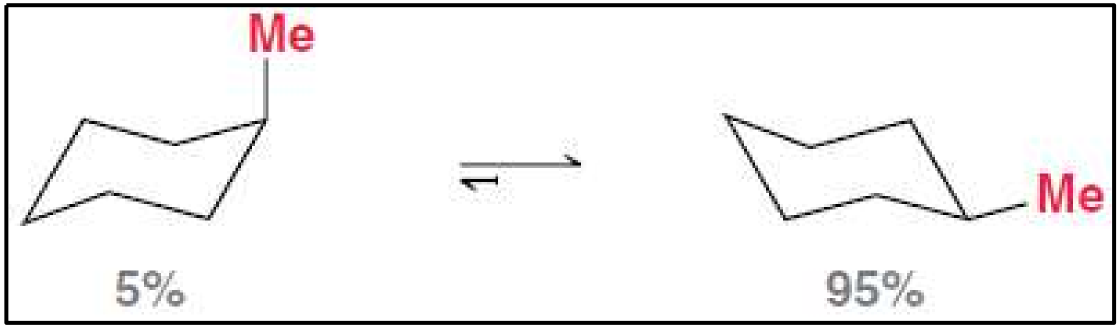
6.6 Comparing the Stability of Chairs

- **If both versions of the CHAIR were equally stable, you would have a 50/50 mixture of axial/equatorial**
- Consider methylcyclohexane



- Why does the equatorial chair dominate the equilibrium?
- Does the axial substituent cause additional angle or torsional strain?

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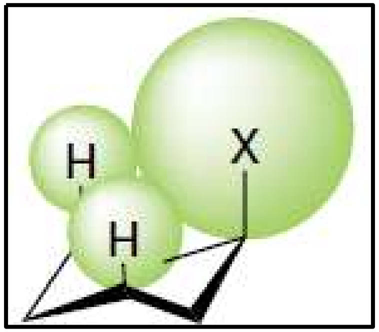
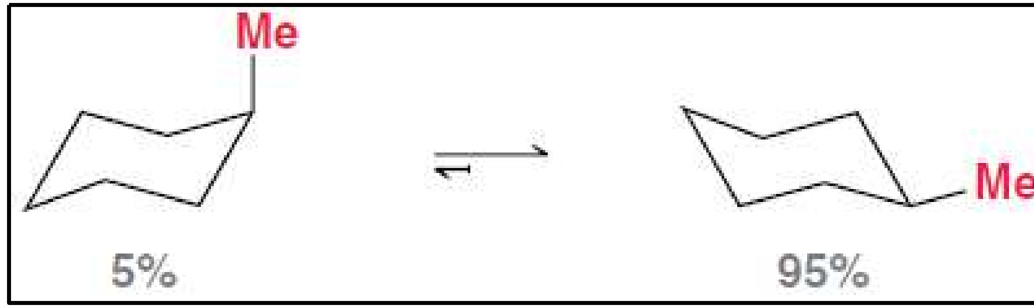
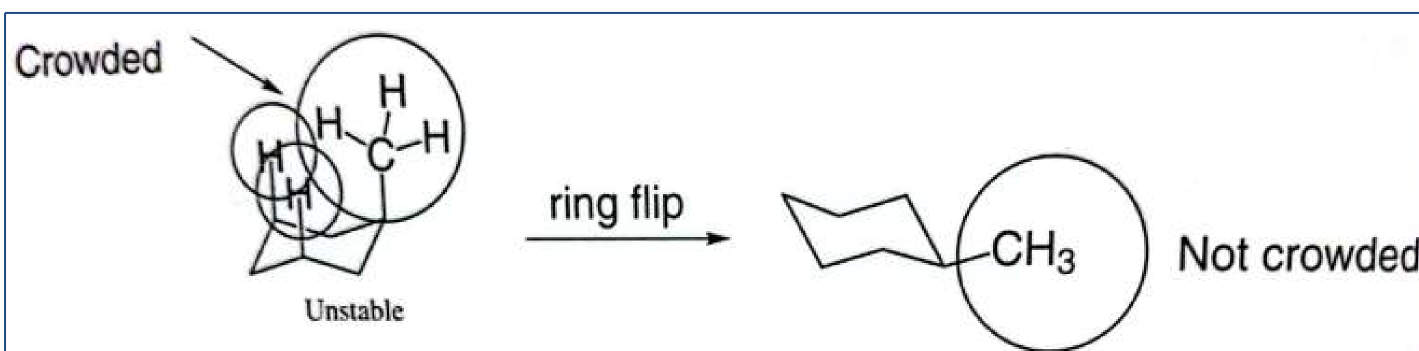
6.6 Comparing the Stability of Chairs

- The axial substituent causes additional steric strain





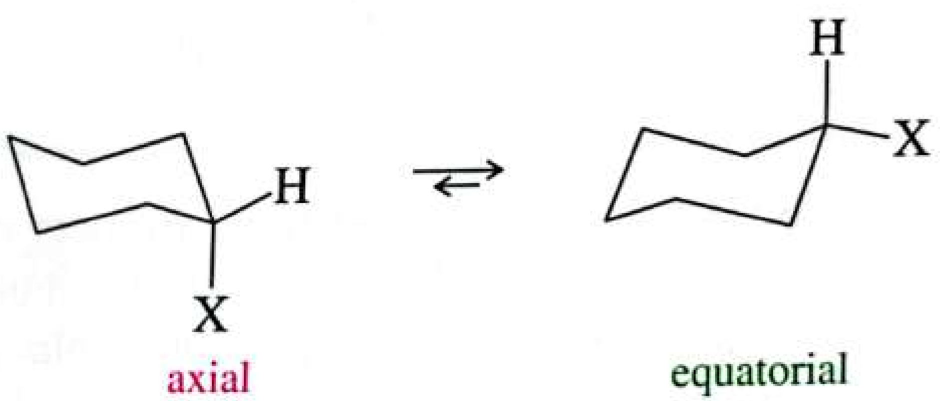
- Such steric crowding is called "**diaxial strain**", specifically, the molecule above has "1,3-diaxial strain". WHY?
  - This "strain" can also be called "**steric hindrance**"
  - you may have to "flip" the ring to see which conformation will be present the most.



6.6 Comparing the Stability of Chairs

The effect of steric hindrance can be calculated. We won't do calculations with these values, but this table shows which atoms/groups experience higher levels of hindrance. You will see on the following slides how to use these to determine stability of chairs.

TABLE 3-6 Energy Differences Between the Axial and Equatorial Conformations of Monosubstituted Cyclohexanes

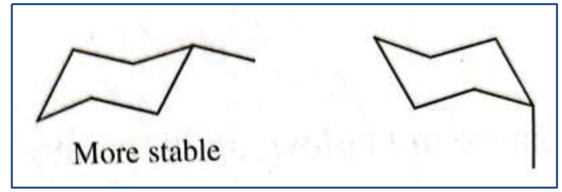


X	ΔG (axial–equatorial) (kJ/mol)
—F	0.8
—CN	0.8
—Cl	2.1
—Br	2.5
—OH	4.1
—COOH	5.9
—CH_3	7.6
—CH_2CH_3	7.9
—$CH(CH_3)_2$	8.8
—$C(CH_3)_3$	23

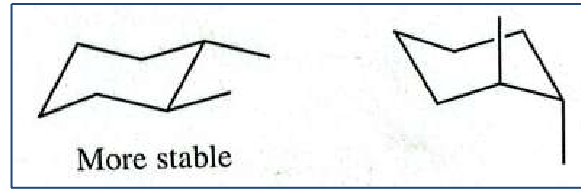
Increasing hindrance in axial positions (↓)

6.6 Comparing the Stability of Chairs

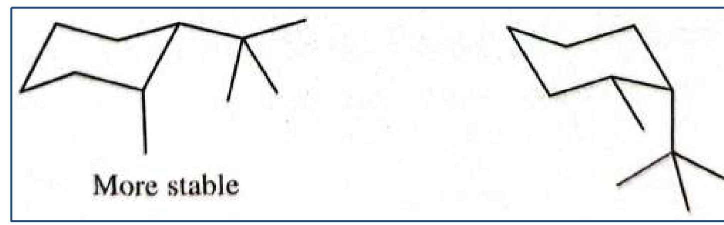
- If you have one group on the ring, the more stable chair will have it in the equatorial position.



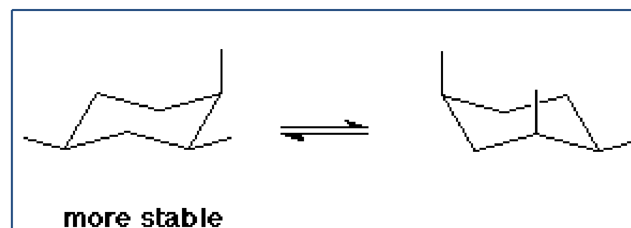
- If you have 2 groups on the ring, its most stable when both groups are in the equatorial position…



  - **If both can't be in the equatorial position**, the larger of the two groups will be more stable in the equatorial position.



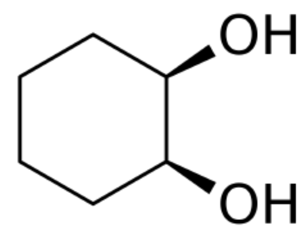
- If you have *more than 2 groups,* use the same logic we used above!



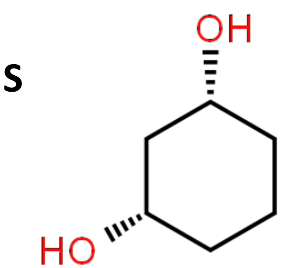
PRACTICE: Go back to where you drew out both chairs on the previous slides for section 6.5 (#1-5 and a-e), **circle the more stable chairs**. If there is a tie, explain why! **CLICK HERE to see the completed slides to practice**
Then, read Klein packet pages 129-133 (section 6.6) and answer questions 6.38-6.45.

6.7 Don’t be Confused by Nomenclature

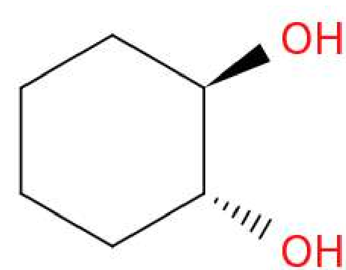
- Some nomenclature can be confusing. We will see terms like “cis and trans” when we don’t have double bonds.
- When we have 2 groups **both** “up” or **both** “down”, we say they are *cis* to each other.



BOTH are CIS

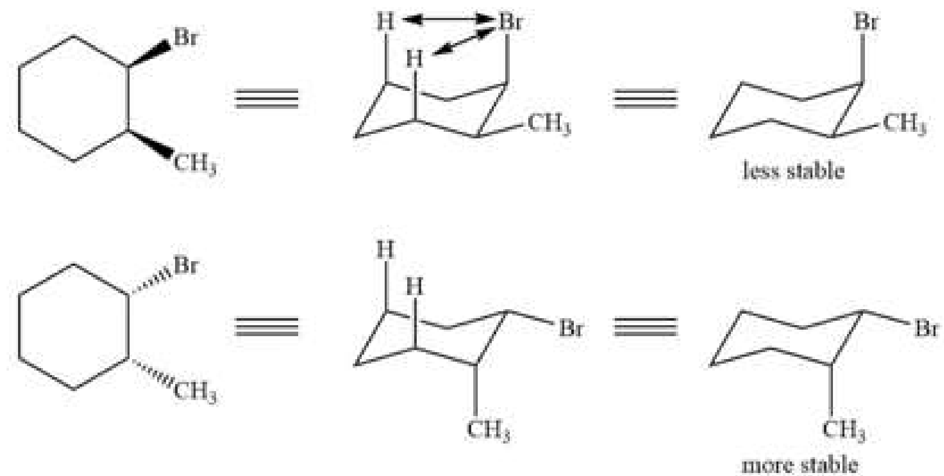


- When we have 2 groups and **one** is “up” and the **other** “down”, we say they are *trans* to each other.
  - Axial/equatorial does not matter here!
  - Remember -ane- means all single bonds

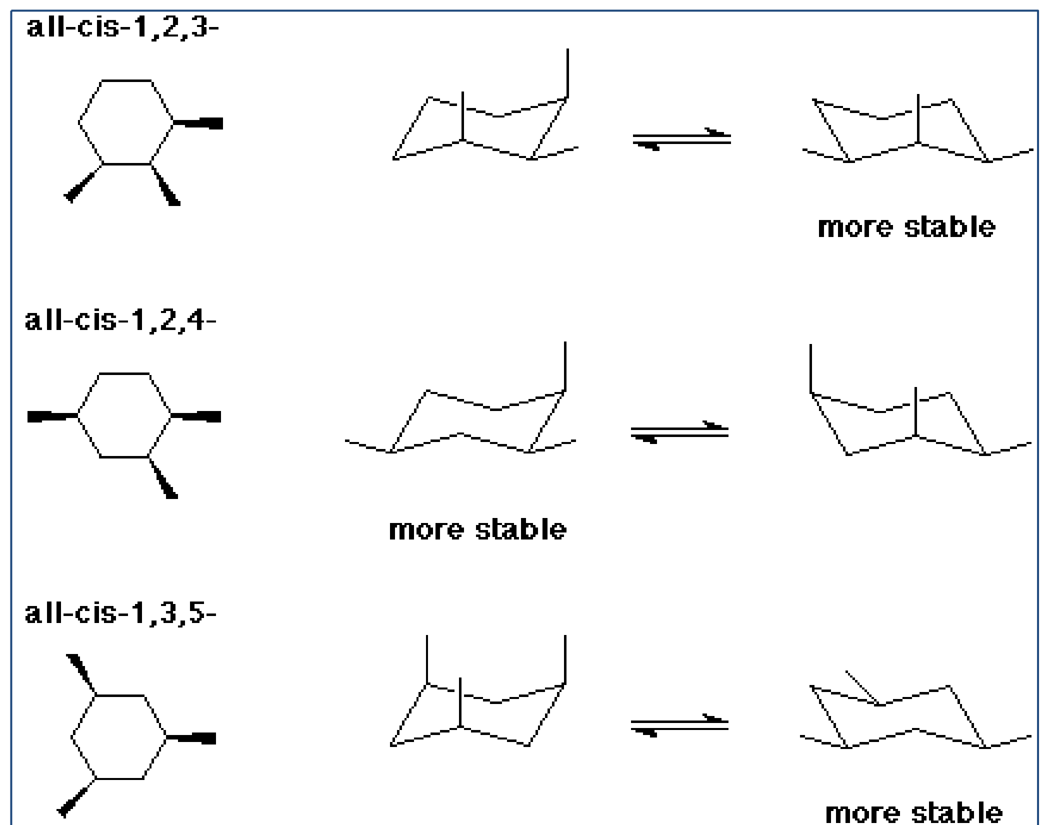


6.7 Don't be Confused by Nomenclature

- Cis and Trans can be used for cylcohexanes that have more than just 2 groups



  - In these examples the groups are all cis to each othe: they would all be on wedges *(or dashes - not shown)*



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6.7 Don’t be Confused by Nomenclature Practice

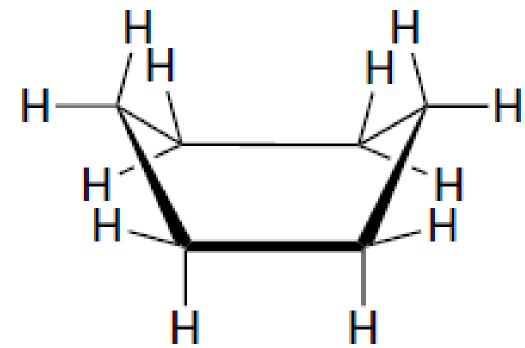
1. Determine if the cis or trans conformation of para-dibromocyclohexane would be more stable. *(Hint: you will want to draw each possibility out, don’t forget about the flipped rings! Once you “get it” you won’t have to do as much work!)*

Click HERE to see the completed slide

READ Page 133 (section 6.7) in your Klein Packet

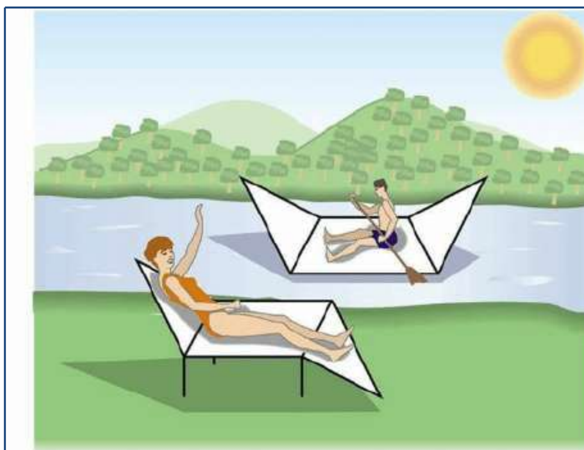
More types of Conformations for Cyclohexanes

- Other conformations of hexane exist but are a bit less stable. Consider **THE BOAT**



1. No angle strain - angles are 109.5°
2. Torsional strain.
   - Use a molecular model to identify all four pairs of eclipsing C-H bonds
   - Draw a Newman projection that illustrates the torsional strain
3. Steric strain – flagpole interactions. WHERE?

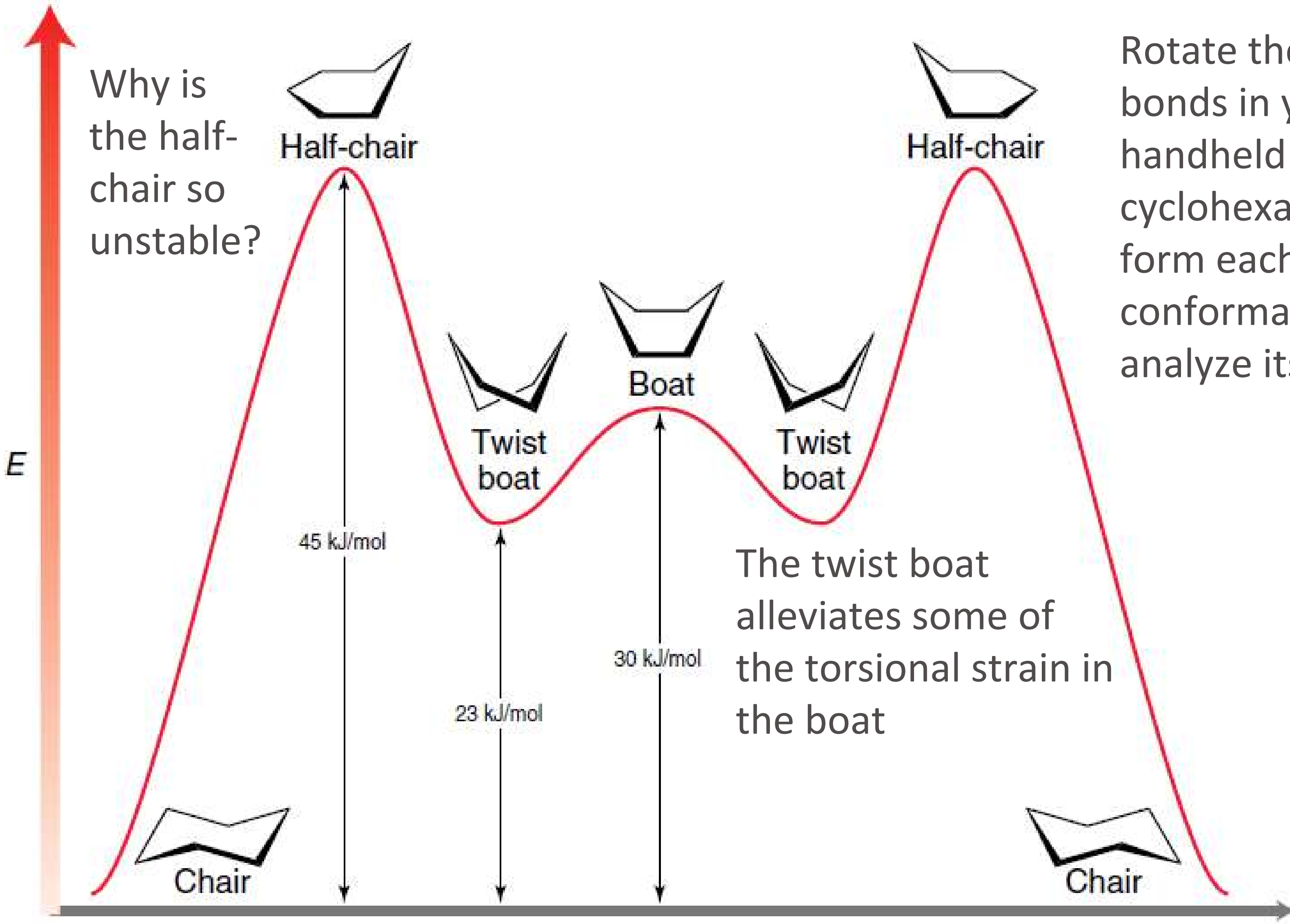
- Why is this conformation called the BOAT?
- You can create a cyclohexane model and create the conformations.



I bet that boat will sink . It is less stable than chair conformation 😂

Cyclohexane Conformations

Why is the half-chair so unstable?



The twist boat alleviates some of the torsional strain in the boat

Rotate the C-C single bonds in your handheld cyclohexane model to form each of the conformations and analyze its energy

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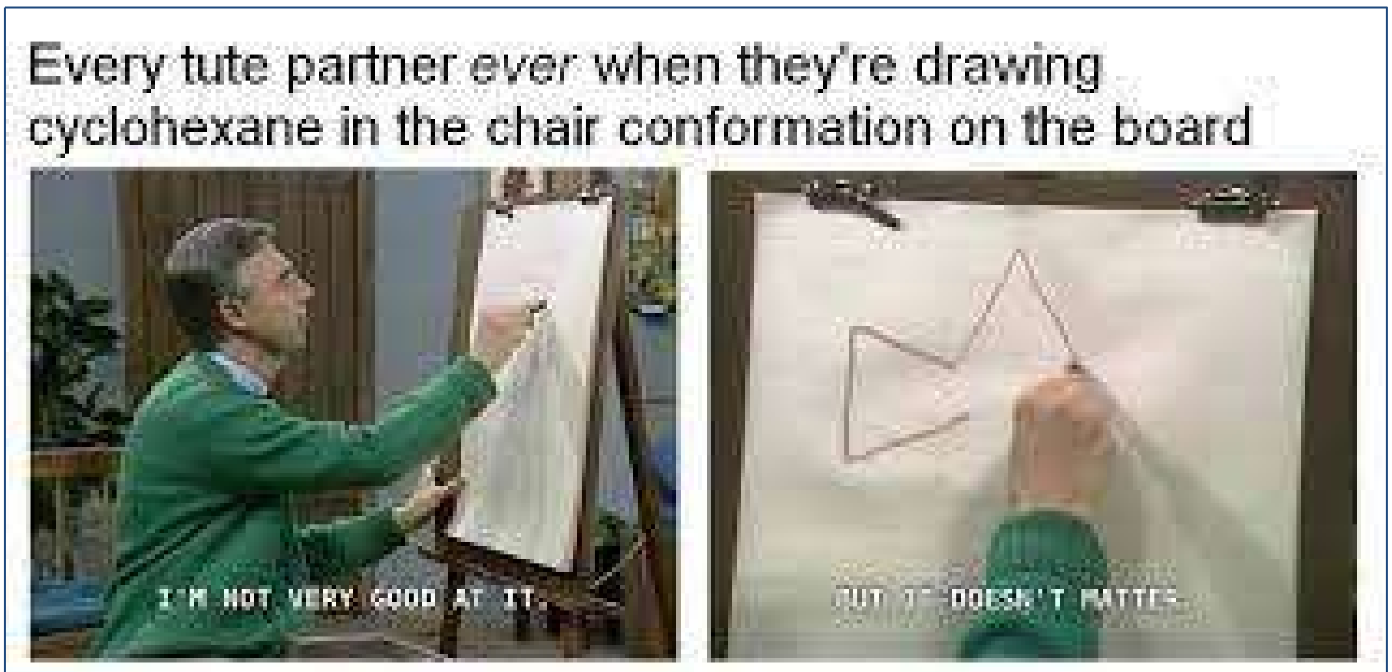
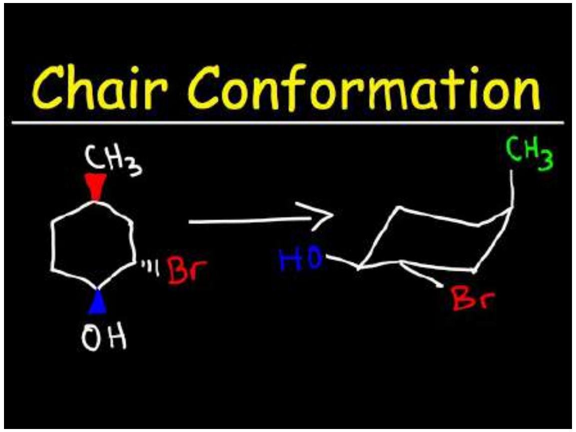
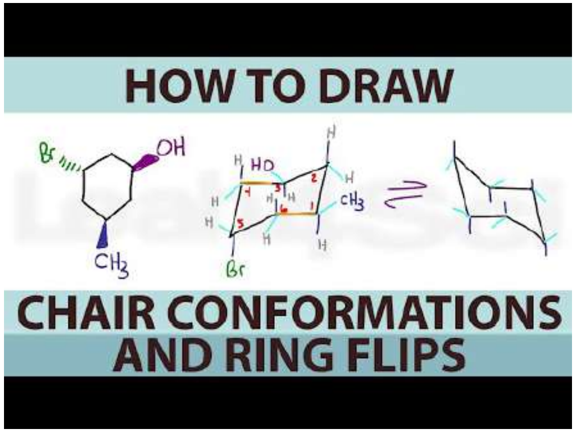
Because we love nerdy memes!



There are extra practice videos embedded in the google slide notes posted on google classroom!

Practice Videos for Chair Conformations!





END of Teacher Slides
Student Slides to Follow

END of Teacher Slides
Student Slides to Follow

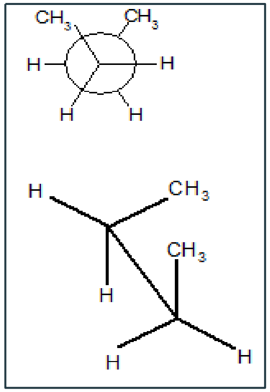
Name: ______________________________

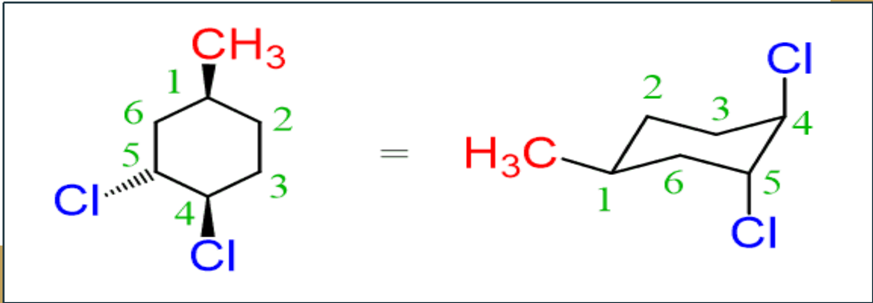
Organic Chemistry Notes
Chapter 6: Conformations
Alkanes, Chairs, and Newman Projections

Chapter 6 Objectives:

Students will be able to:

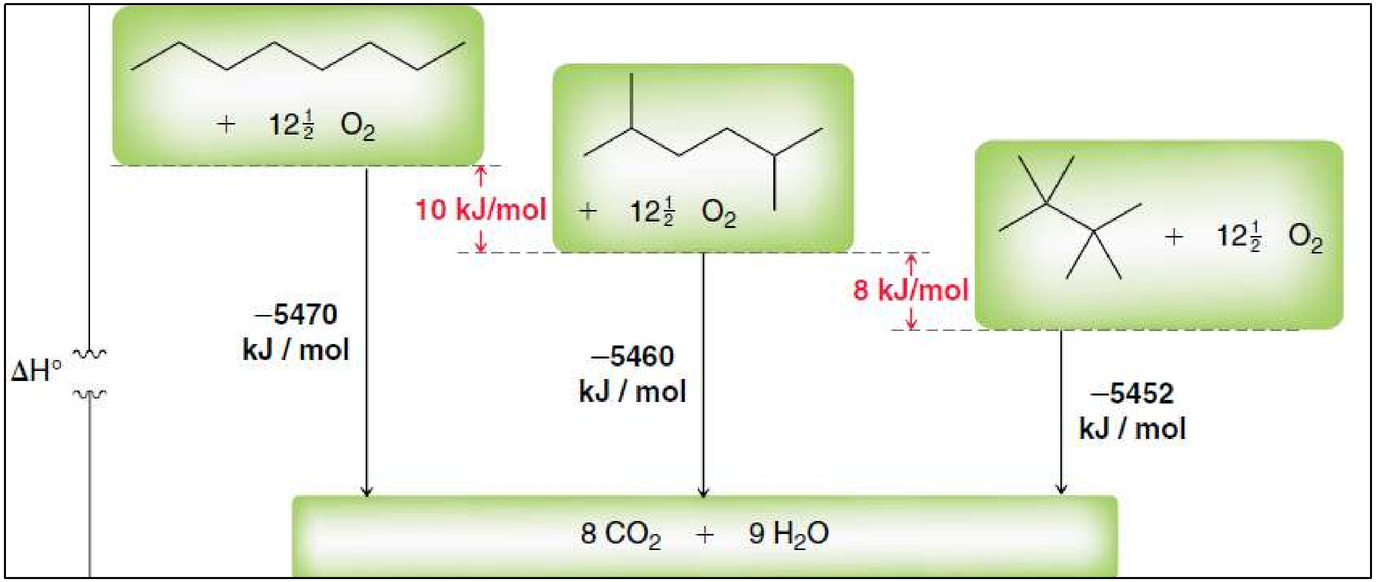
1. Describe the need for conformation analysis as it relates to alkanes.
2. Draw Newman Projections for various alkanes.
3. Rotate and assess stability of Newman Projections.
4. Draw chair conformations of cyclohexanes, including all axial and equatorial positions.
5. Flip and assess the stability of various chair conformations.





6.0 Relative Stability of Isomers

- To rationalize and predict the outcomes of chemical reactions, it is helpful to assess stability of compounds
- Remember: ___________ = ______ potential energy = _____________________ = ________________ will be released upon reacting
- If you drove a car today, what type of chemical reaction with alkanes did you perform?
- What is the general reaction equation for the combustion of octane?
- Com



6.0 Sources and Uses of Alkanes

- __________________, which literally means ______________ is the main source of alkanes
- Petroleum is a mixture of hundreds of hydrocarbons, mostly alkanes with varying numbers of carbons and varying degrees of branching
- The alkanes in petroleum with 5 to 12 carbons per molecule are most valuable, and they can be separated from the rest of the oil by distillation
- HOW does distillation work?

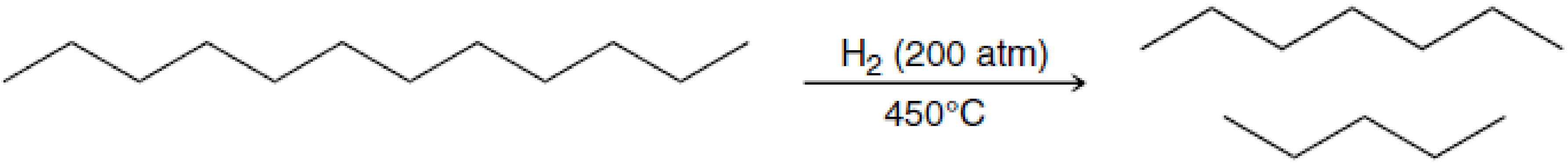
- Table 4.5 shows the various components of petroleum
- The gasoline fraction of crude oil only makes up about 19%

TABLE 4.5 INDUSTRIAL USES OF PETROLEUM FRACTIONS

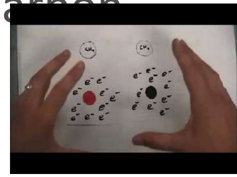
BOILING RANGE OF FRACTION (° C)	NUMBER OF CARBON ATOMS IN MOLECULES	USE
Below 20	$C_1 - C_4$	Natural gas, petrochemicals, plastics
20 – 100	$C_5 - C_7$	Solvents
40 – 200	$C_5 - C_{12}$	Gasoline
175 – 300	$C_{12} - C_{18}$	Kerosene, jet fuel
275 – 400	C_{12} and higher	Heating oil, diesel
Nonvolatile liquids	C_{20} and higher	Lubricating oil, grease
Nonvolatile solids	C_{20} and higher	Wax, asphalt, tar

6.0 Sources and Uses of Alkanes

- Gasoline is a mixture of straight, branched, and aromatic hydrocarbons (5-12 carbons in size)
- Large alkanes can be broken down into smaller molecules by *Cracking*

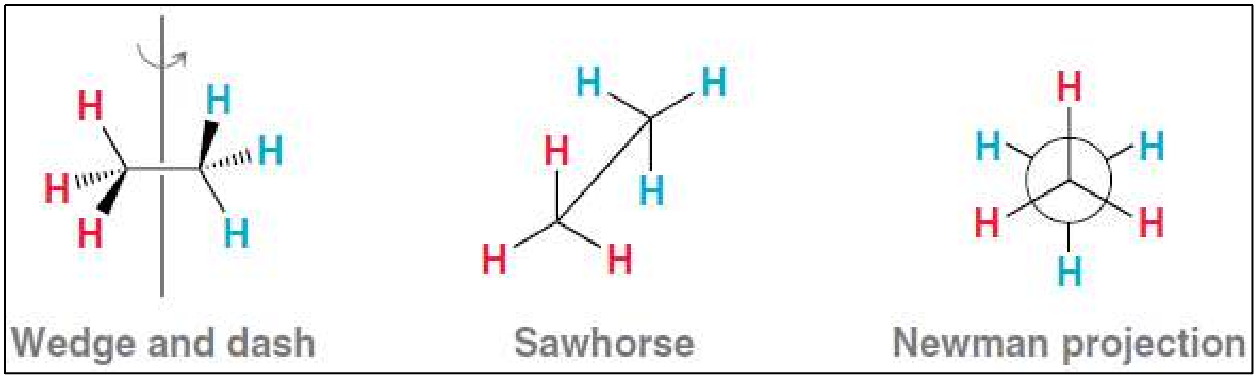


- Straight chain alkanes can be converted into branched alkanes and aromatic compounds through *Reforming*
- After using these processes, the yield of gasoline is about 47% rather than 19%
- **At room temperature:**
  - Small alkanes with 1-4 carbons are gasses
  - Medium size alkanes with 5-12 carbons are liquids
  - Large alkanes with 13-20 carbons are oils
  - Extra large alkanes with 20-100 carbons are solids like tar and wax
  - Super-sized alkanes called polymers can have thousands or millions of carbon atoms in each molecule
- What type of properties would y pect such polymers to possess?

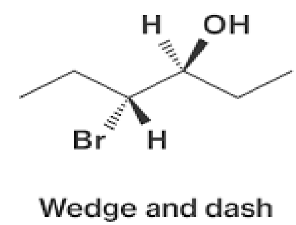


6.1 Newman Projections

- We know that ______________________________
- Different rotational states are called _______________
- 3D Rotational conformations are difficult to represent on a 2D paper. *It's useful to make a molecular model to help you visualize the structures*
- Here are three ways to represent ethane



1. It doesn't matter if the wedge is on the left or right

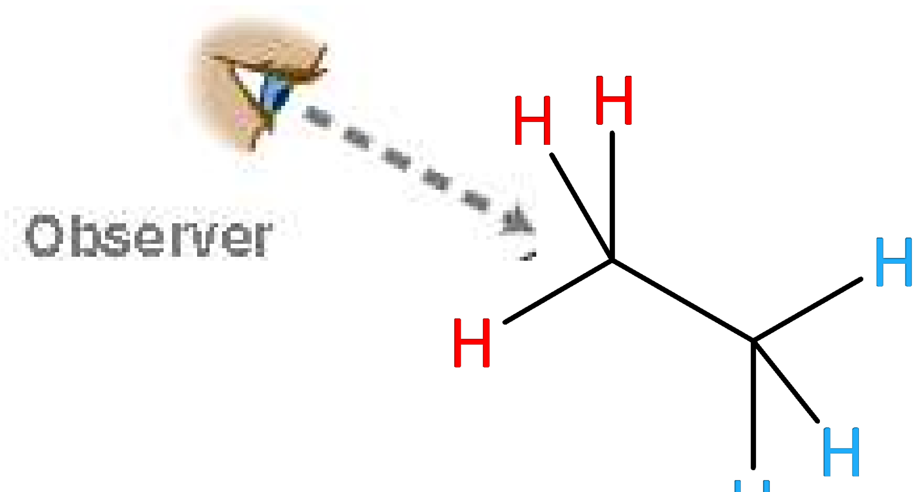


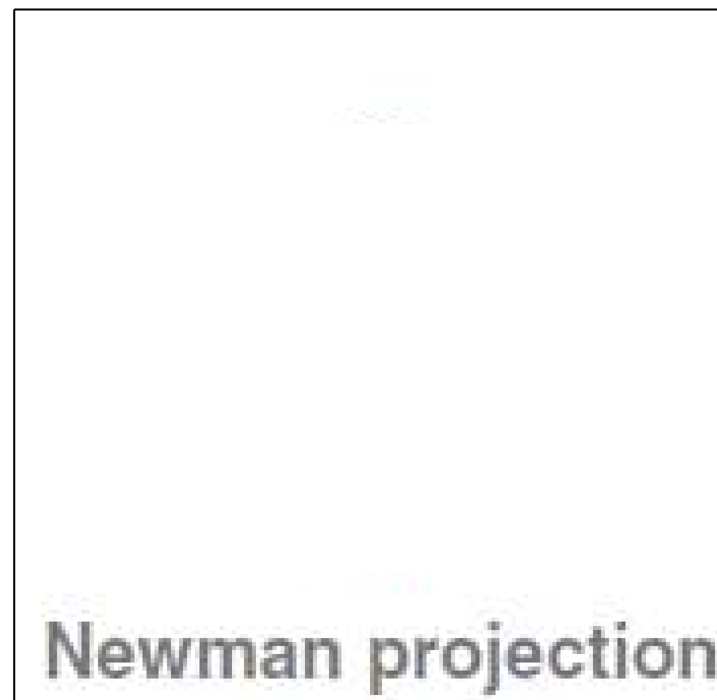
1. EACH tetrahedral carbon will have:
    - ____ straight bonds (in-plane of paper)
    - ____ wedge (coming towards you)
    - ____ dash (going away from you)

1. Sometimes we won't show all of the wedges/dashes, especially if they are H's attached to carbons

6.1 Newman Projections

- Look directly down the C-C single bond axis. This is where it is especially helpful to have a model
- The front carbon should eclipse the single bond and the carbon behind it
- Show the front carbon as a _______ and the back carbon as a _________ behind it





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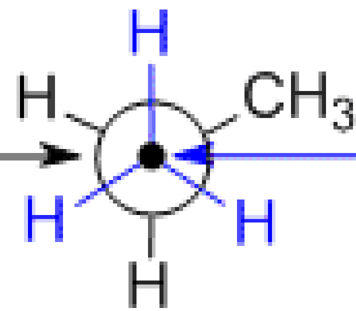
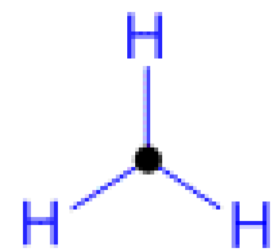
6.1 How to Draw Newman Projections

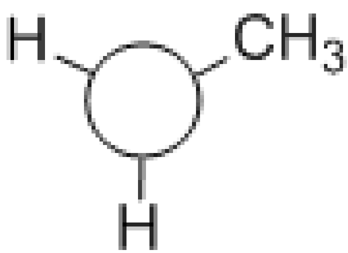
The "circle" defines the **back** carbon atom and the groups attached to it



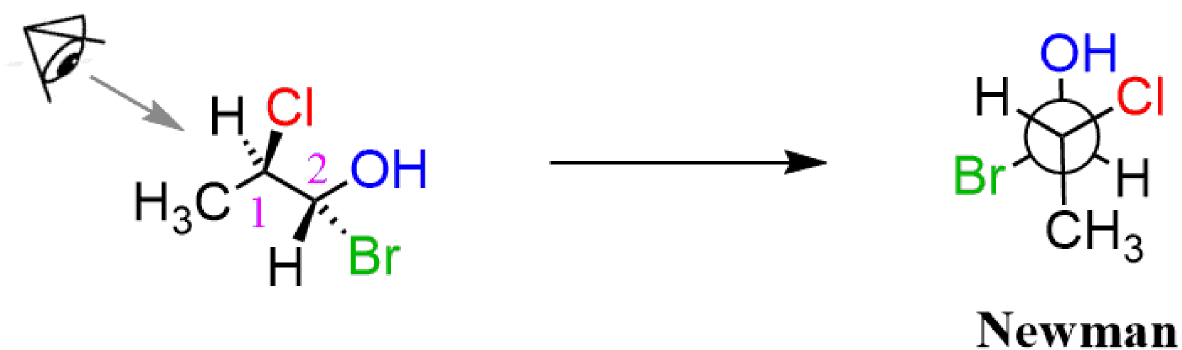
The "dot" defines the **front** carbon atom and the groups attached to it



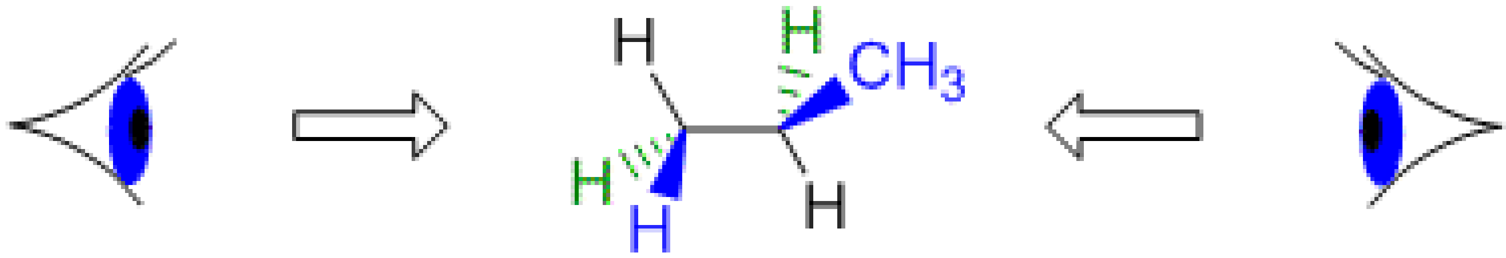
back carbon only



front carbon only



Newman Projections are all about PERSPECTIVE!

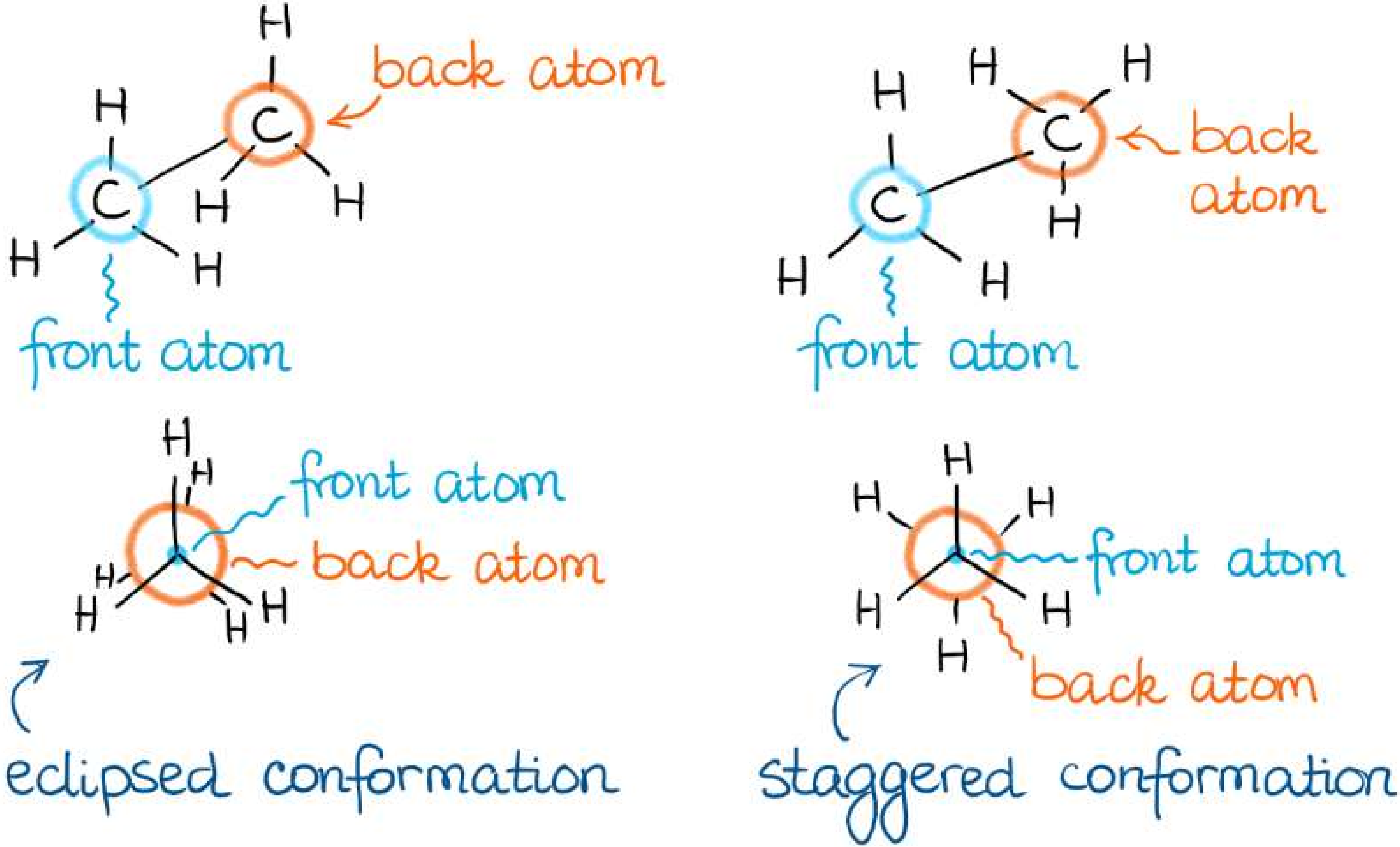


remember **hashes** are in to the page (back) and **wedges** are out of the page (forward)

when viewed from the left (methyl group on back C and to the right)

when viewed from the right (methyl group on the front C and to the left)

There will usually be an arrow or eyes telling you which way to view your molecule from.



Short-Cuts we may see…

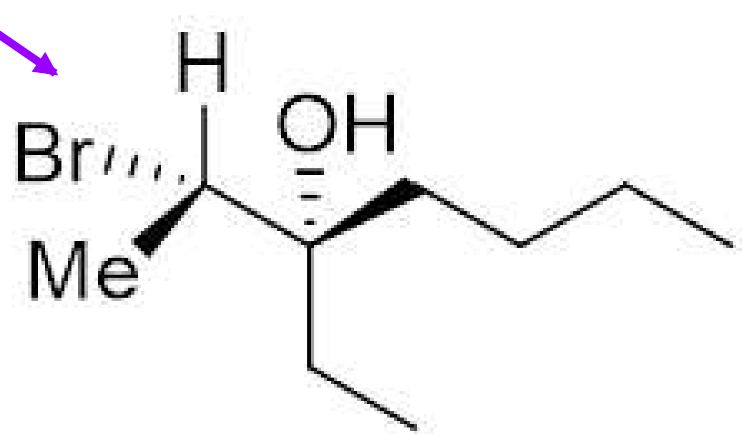
CH_3 = methyl = ______

CH_2CH_3 = ethyl = ______

$CH_2CH_2CH_3$ = propyl = _______

$CH_2CH_2CH_2CH_3$ = butyl = _________________

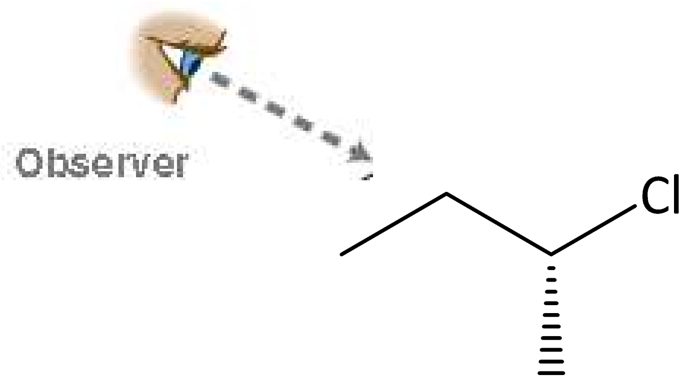
**There are many more - just try to reason them out!*



This wedge/dash drawing is the same as the Newman Projection

6.1 Newman Projections

- Draw a Newman projection for the following molecule



- How would it look if the observer were viewing it from the opposite direction?

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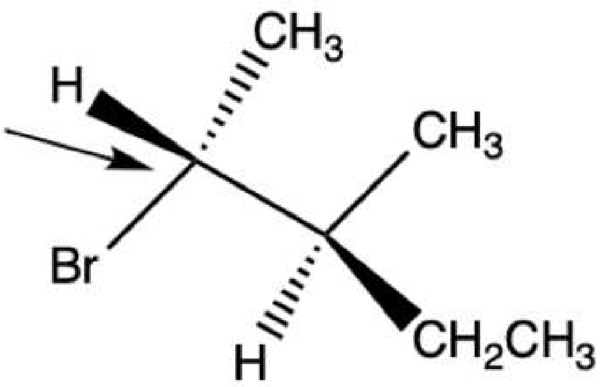
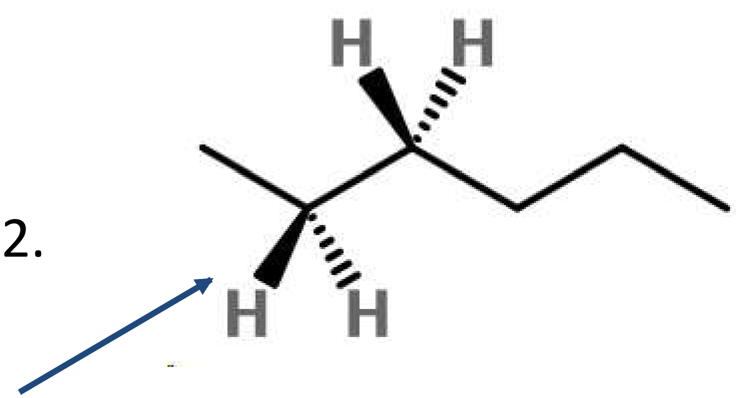
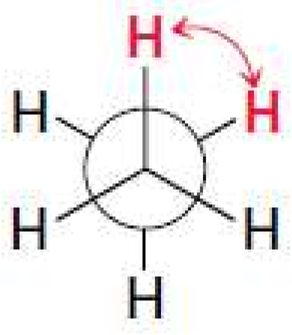
Let's Practice! Draw the Newman projection as it is shown (don't rotate yet!)

1.  =

2. 

6.2 Rotational Conformations

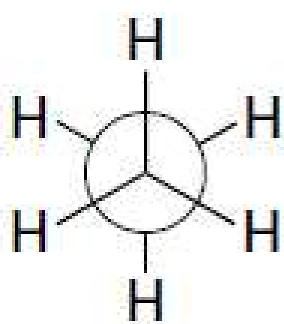
- What is the angle between H atoms on the same carbon? In the Newman projection it looks like 120°.
- Does the angle affect stability? WHY? Think about areas of *high electron density repelling*
- The angle between H atoms on adjacent carbons is called a dihedral or ____________ angle. It is 60° in the molecule below



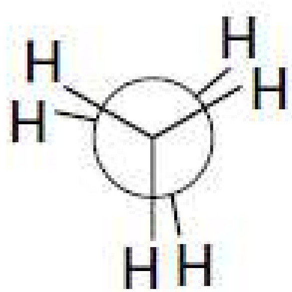
Dihedral angle = 60°

6.2 Rotational Conformations

- If ethane were to rotate 60° about the C-C bond, the the H atoms on adjacent carbons eclipse one another
- Compare the stability of the _______________ and _______________ conformations based on the repulsion of areas of high electron density



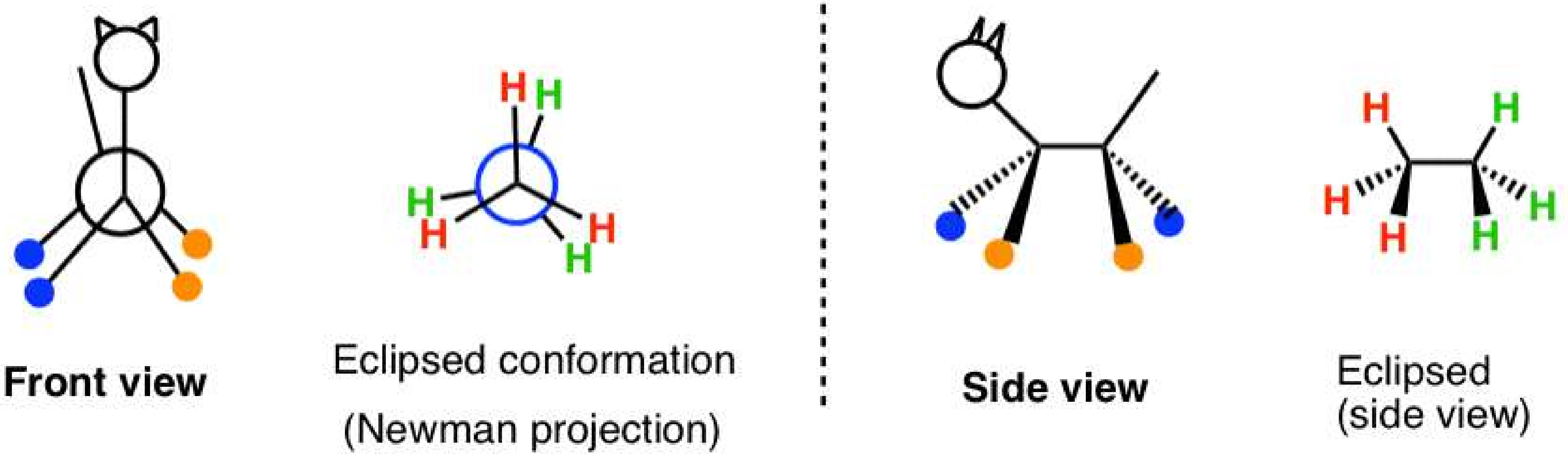
Staggered conformation
Lowest in energy



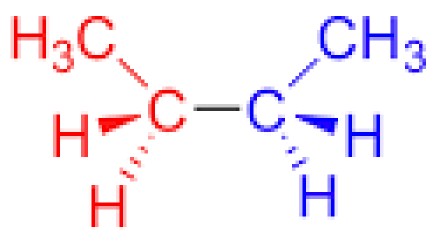
Eclipsed conformation
Highest in energy

- What other conformations are possible?

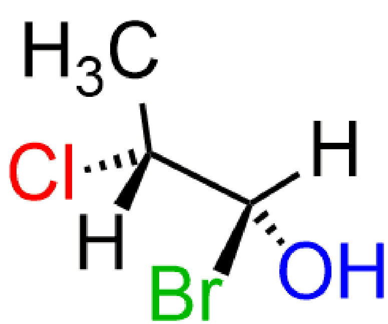
Sometimes the molecules given have an "eclipsed" formation



3.

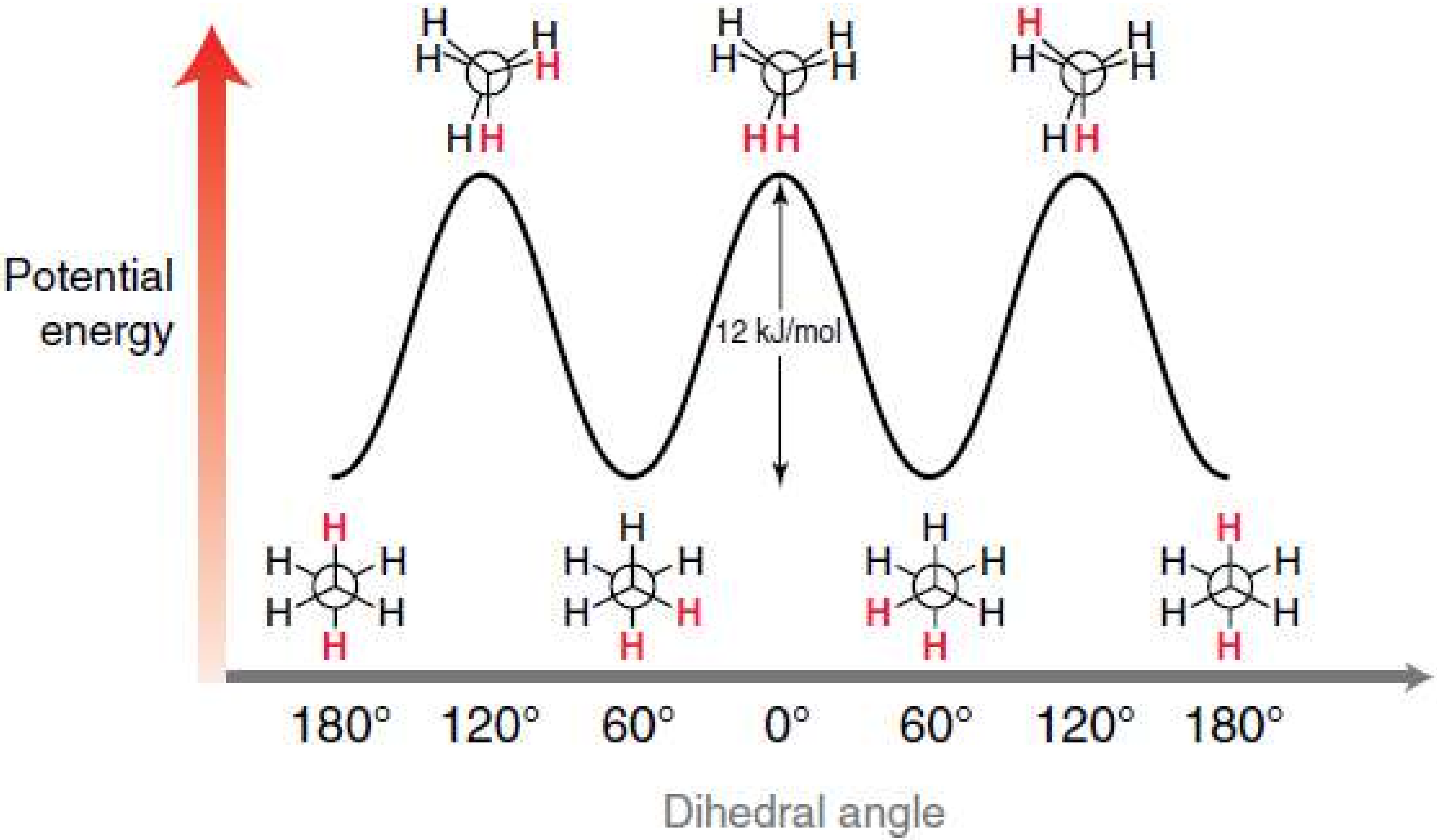


4.



6.2 Rotational Conformations

- Consider a complete 360° rotation about the C-C bond



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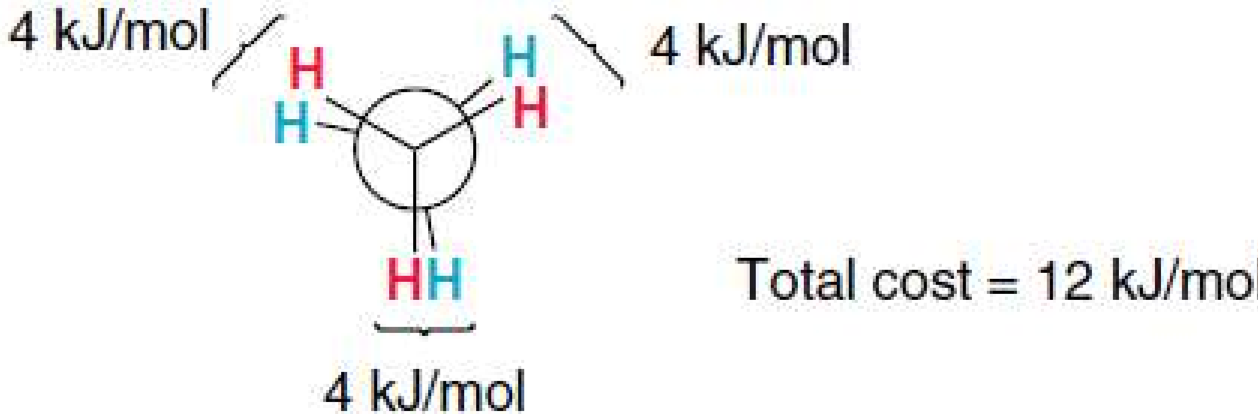
6.2 Rotational Conformations

- The difference in energy between the staggered and eclipsed conformations is called ____________________
- *With a difference of 12 kJ/mol in stability, at room temperature, 99% of the molecules will be in the staggered conformation*



- How would the ratio change at a higher temperature?

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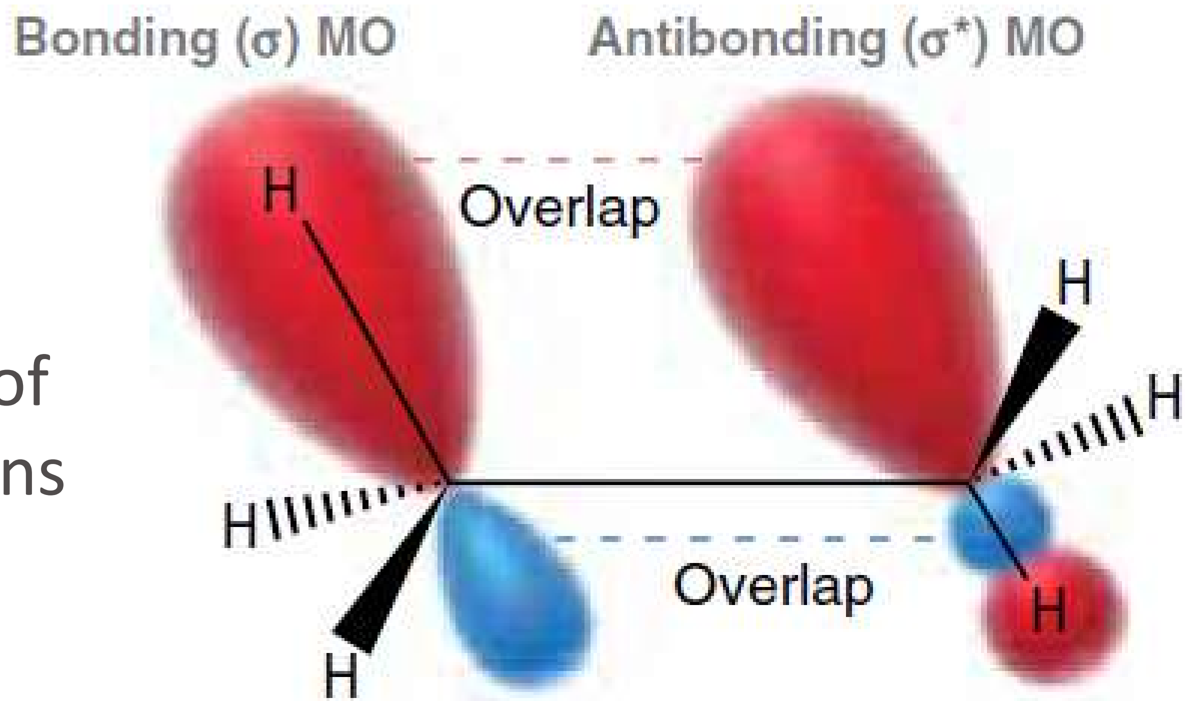
6.2 Rotational Conformations

- **Torsional strain** can also be explained using molecular orbital theory

- In the staggered conformation, the bonding and antibonding MOs of neighboring carbons overlap



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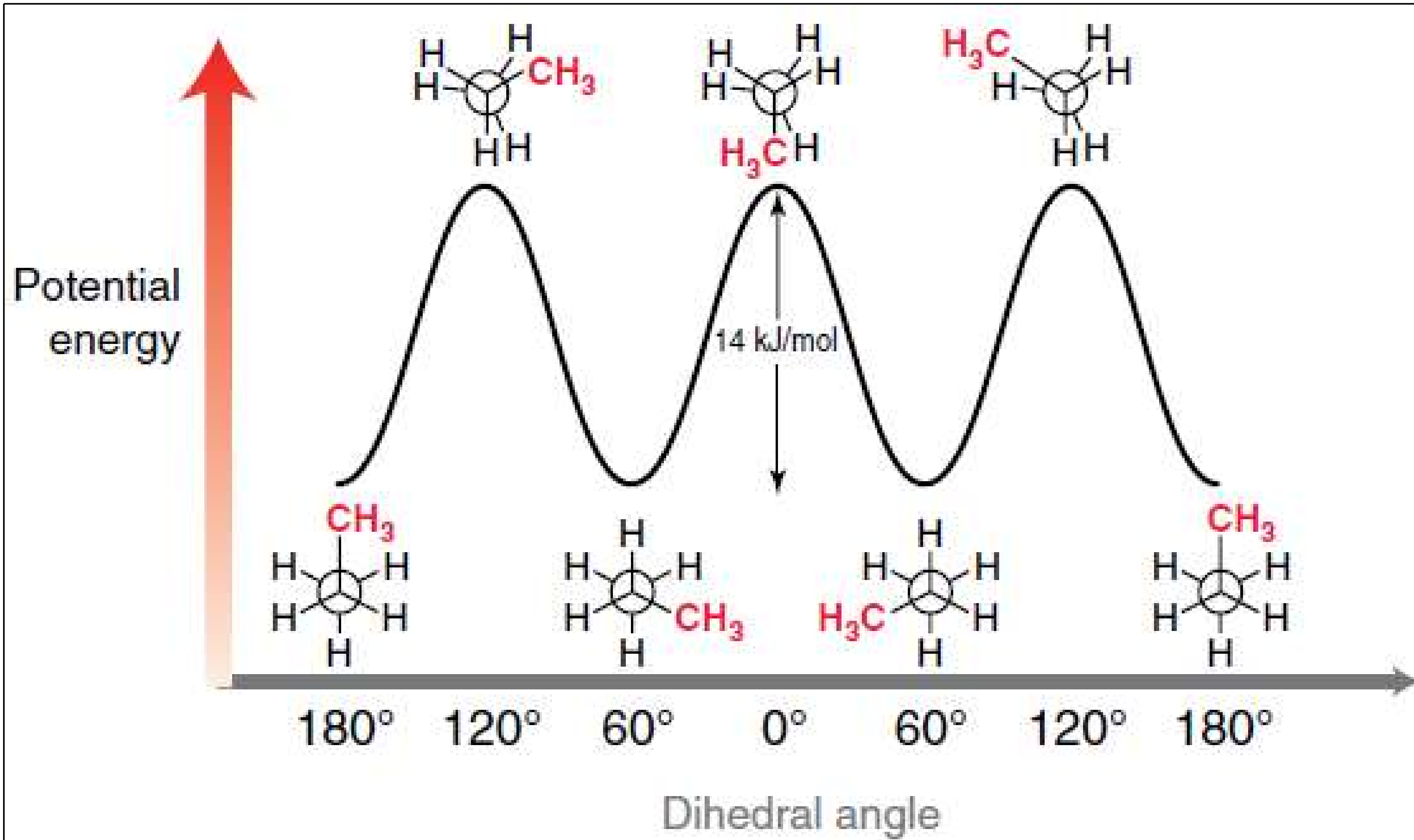
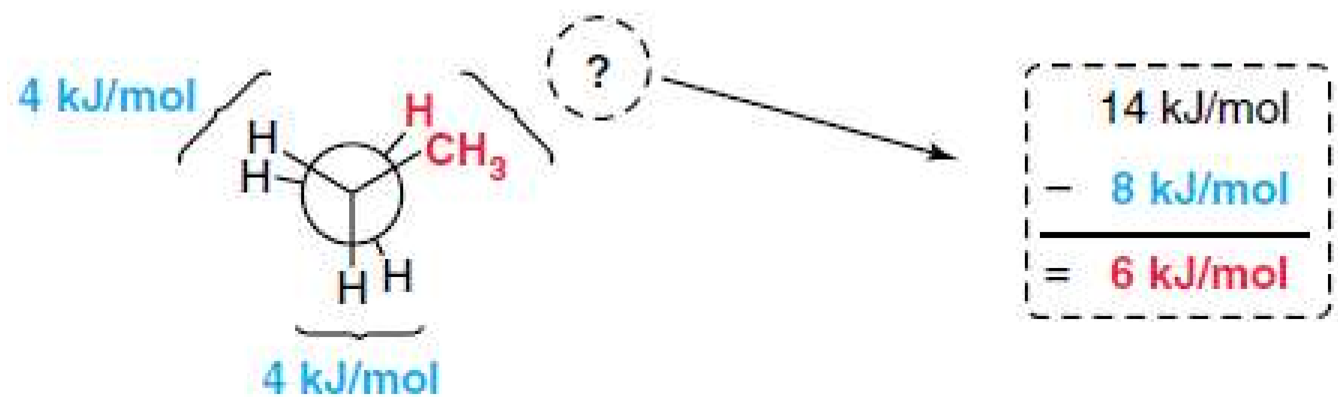
6.2 Rotational Conformations

- The analysis of **torsional strain** for propane shows a very similar situation



6.2 Rotational Conformations

- The **torsional strain** for propane is 14 kJ/mol, which is 2 kJ/mol more than for ethane
- If each H-----H eclipsing interaction costs 4 kJ/mol of stability, that total can be subtracted from the total 14 kJ/mol to calculate the contribution of a CH_3-----H eclipsing interaction



- Practice with conceptual checkpoint 4.19

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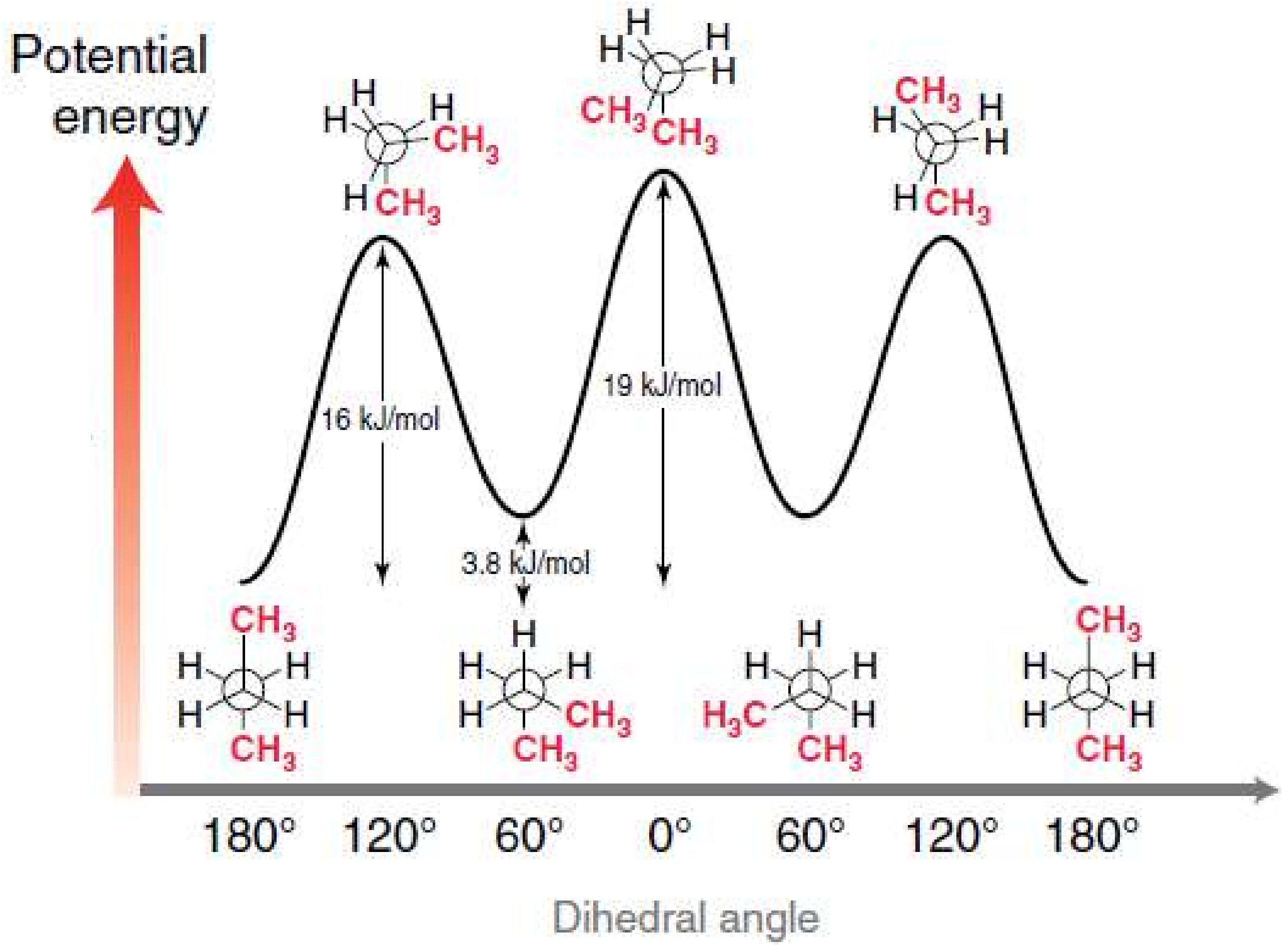
6.2 Butane's Conformations

- The analysis of **torsional strain** for butane shows more variation

- Note that there are multiple staggered conformations and multiple eclipsed conformations



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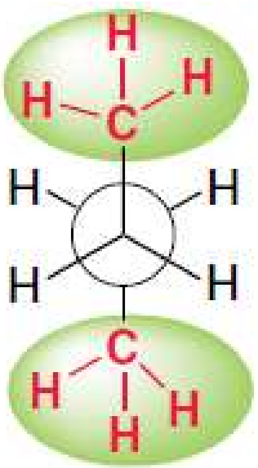
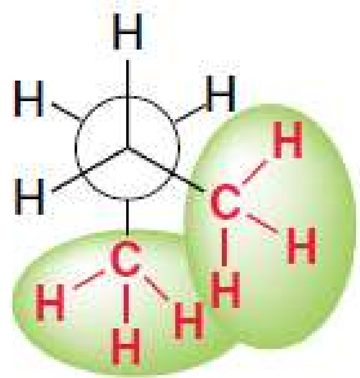
6.2 Butane's Conformations

- The stability of the different staggered conformations differs by 3.8 kJ/mol
- The anti conformation has less steric hindrance.



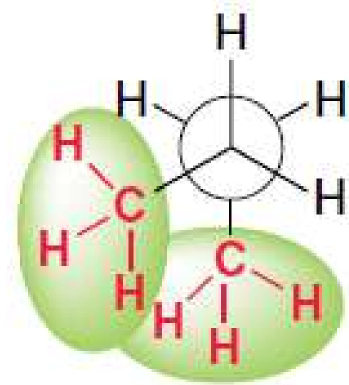
Anti

Methyl groups are farthest apart



Gauche

Methyl groups experience a gauche interaction



Gauche

Methyl groups experience a gauche interaction

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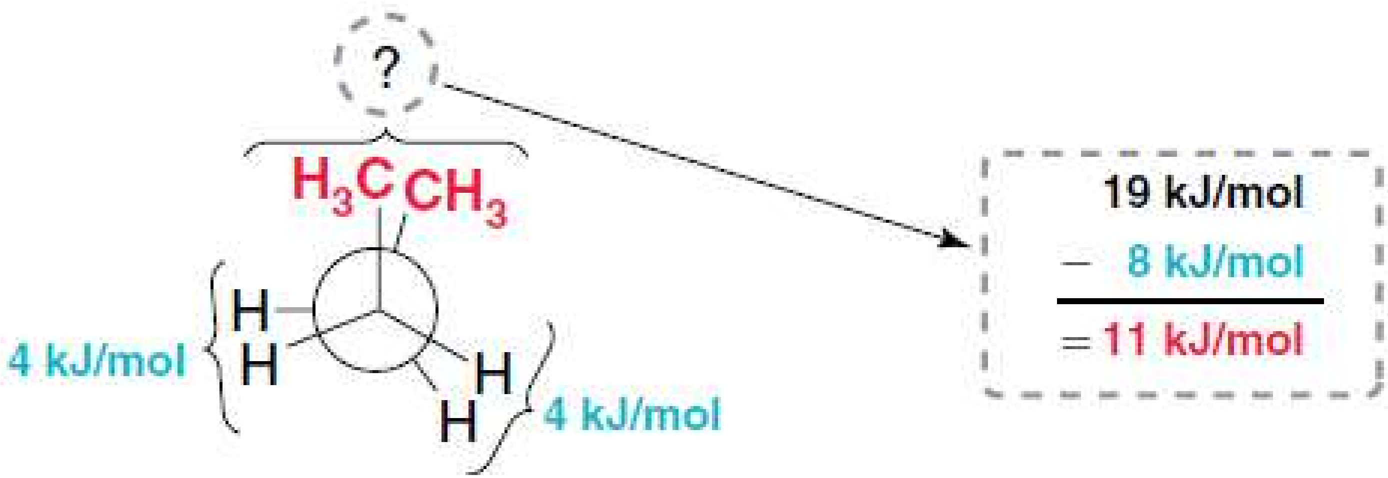
6.2 Butane's Conformations

- The least stable conformation results when the methyl groups eclipse one another



- Each CH_3-----CH_3 **eclipsing** interaction accounts for 11 kJ/mol of energy (torsional and steric strain).

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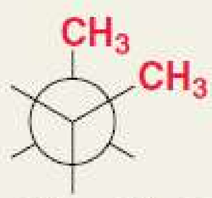
6.2 Butane's Conformations

- The values in table 4.6 can be used to predict relative energies for various conformations

*We don't have to do this for regular points in HS!

INTERACTION	TYPE OF STRAIN	ENERGY COST (KJ/MOL)
 H—H Eclipsed	Torsional strain	4
 CH_3—H Eclipsed	Torsional strain	6
 CH_3—CH_3 Eclipsed	Torsional strain + steric hindrance	11
 CH_3—CH_3 Gauche	Steric hindrance	3.8

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6.2 Rotational Conformations

- Draw a Newman projection for the highest and lowest energy conformations for 2,2,3,5,5-pentamethylhexane from C3 to C4. *(you will have to rotate the bonds)*

Recap the Stability of Newman Projections

Staggered		Eclipsed
Anti	Gauche	
Most Stable	**Stable**	**Least Stable**

Extra Practice

Draw Newman projections for each of the following situations.

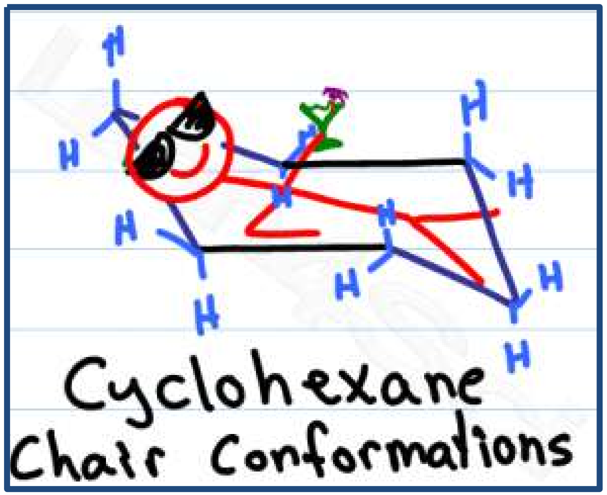
1. The <u>highest</u> energy conformation of 3-methylnonane along the C4 to C5 bond axis

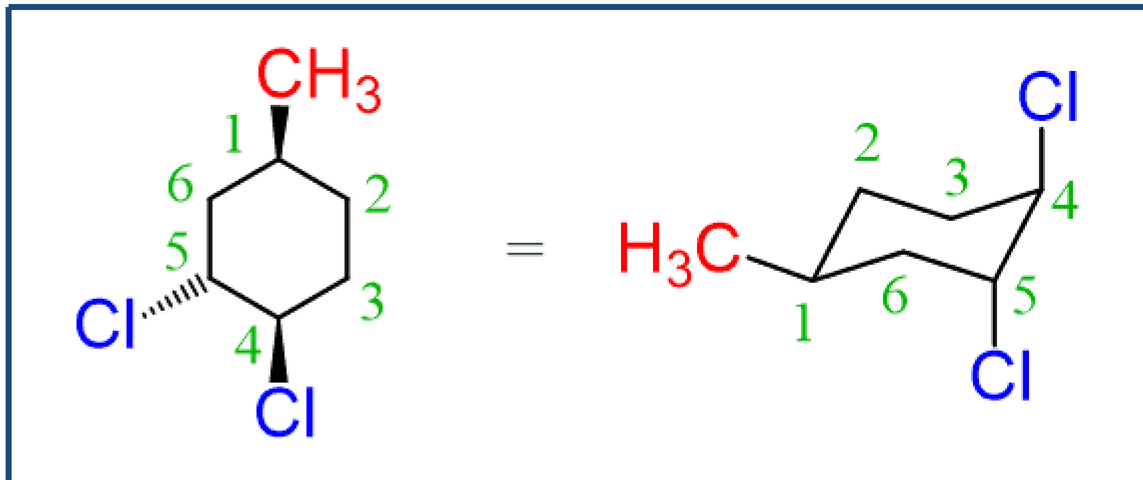
1. The <u>lowest</u> energy conformation of trans-1-bromo-2-methylhexane along the C1 to C2 axis

Name: ______________________________________

Chapter 6 - Part II

Chair Conformations

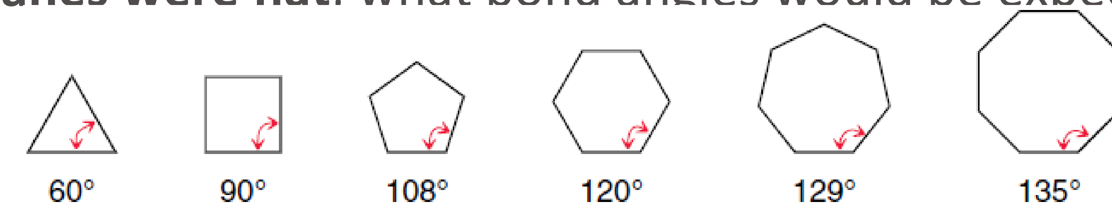




Intro Crash Course Organic Chemistry Video for cycloalkanes

6.3 Cyclic Alkanes

- Carbon atoms in alkanes are sp^3 hybridized
  - What bond angles are optimal for such carbons?
- **If cycloalkanes were flat**, what bond angles would be expected?



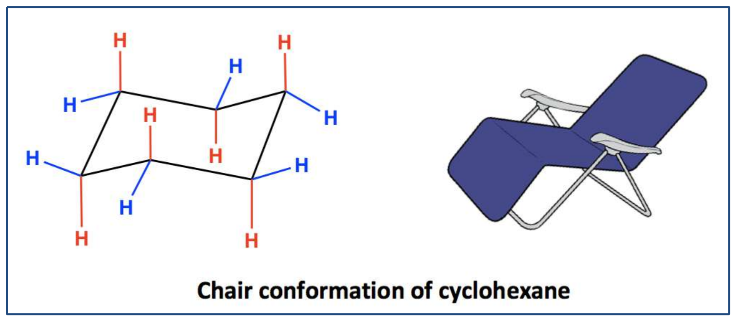
- To optimize the bond angles, most cycloa stable conformation
- **Build a cyclohexane without the hydrogens**
- Why are heats of combustion reported per CH_2 group?
- Considering the data in the table which ring has the least **ring strain**?

CYCLOALKANE	NUMBER OF CH_2 GROUPS	HEAT OF COMBUSTION PER CH_2 GROUP (KJ / MOL)
Cyclopropane	3	697
Cyclobutane	4	680
Cyclopentane	5	658
Cyclohexane	6	653
Cycloheptane	7	657
Cyclooctane	8	658
Cyclononane	9	659
Cyclodecane	10	659
Cycloundecane	11	661
Cyclododecane	12	654

6.3 Cyclohexane

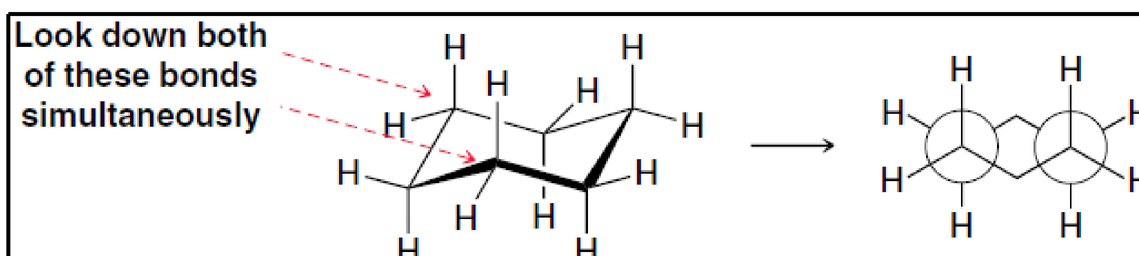
- Cyclohexane is considered to have ZERO ring strain in its optimal conformation, _______________
  1. No angle strain - angles must be 109.5°
  2. No torsional strain - all adjacent C-H bonds must be ______________

_________________ are vertical, ___________________ go around the outside like the equator. (or a tutu!)



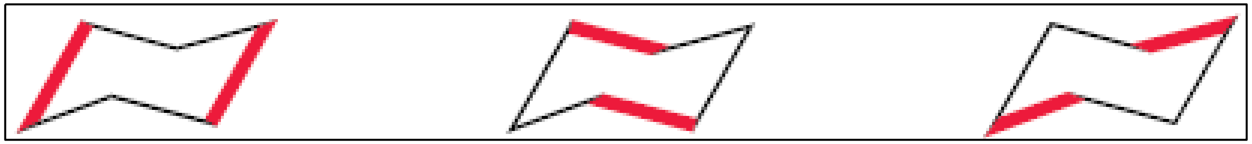
- Chairs can be drawn like 2 Newman Projections, but we don't often to this in HS organic chemistry.
- Add the H's on to your carbon cyclohexane to create the chair. Look down the planes like in the picture below:

Chairs & Newman Projections



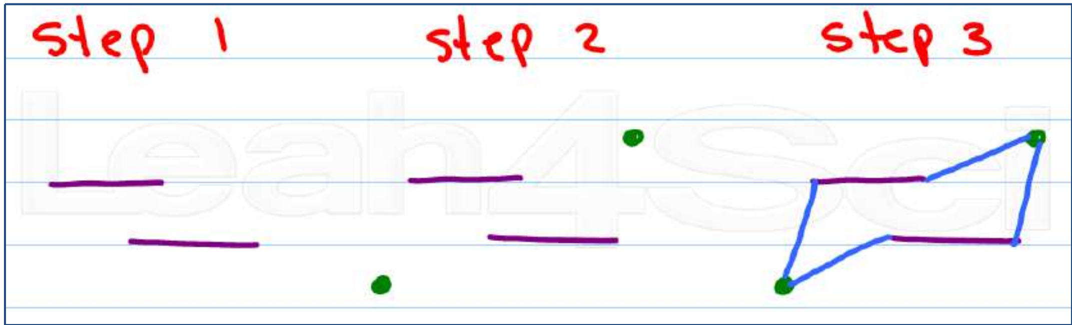
6.3 Drawing Chairs

- **It is critical to draw a CHAIR properly.** Use three sets of parallel lines



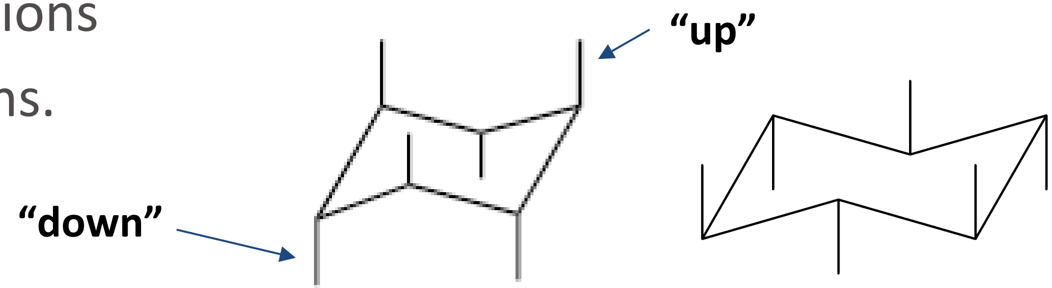
- Let's Practice in the space below! *Draw at least 6 chairs!*

You can also use this "hack" to draw your "forward" chairs!



6.3 Drawing Axial Positions

- SIX of the atoms attached to the chair are **axial**. Axial groups point straight up and down alternating around the ring. *Mrs. H likes to start with what she calls "carbon #1" it is vertically "up".*
- Practice drawing 3 chairs with axial positions in the space below
  - there are 3 axial "up" positions
  - and 3 axial "down" positions.

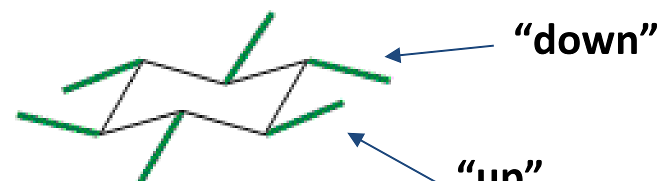


Correct Incorrect

6.3 Drawing Equatorial Positions

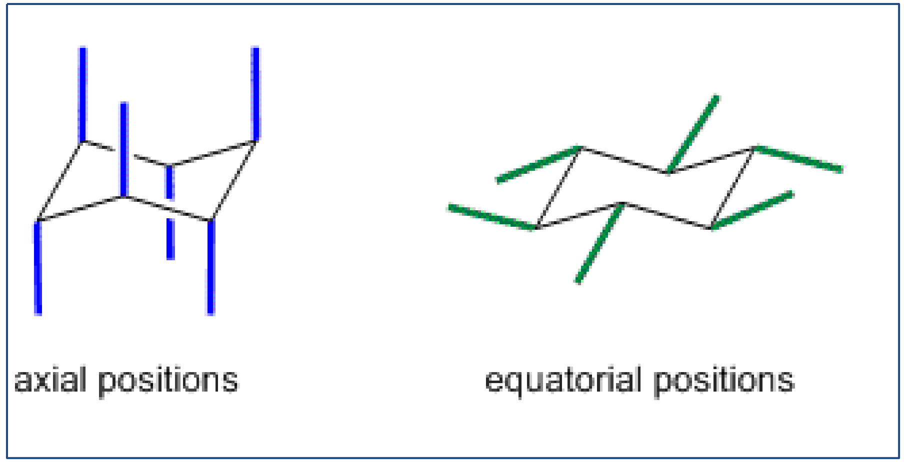
- SIX of the atoms attached to the chair are **equatorial**. Equatorial substituents are positioned at angles parallel to the sets of parallel lines making up the chair itself. *Mrs. H likes to start with what she calls "carbon #1" it is equatorial "down", it will alternate between "up" and "down" just like the axial positions.*

- Practice drawing 3 chairs with equatorial positions in the space below
  - there are 3 equatorial "up" positions
  - and 3 equatorial "down" positions.

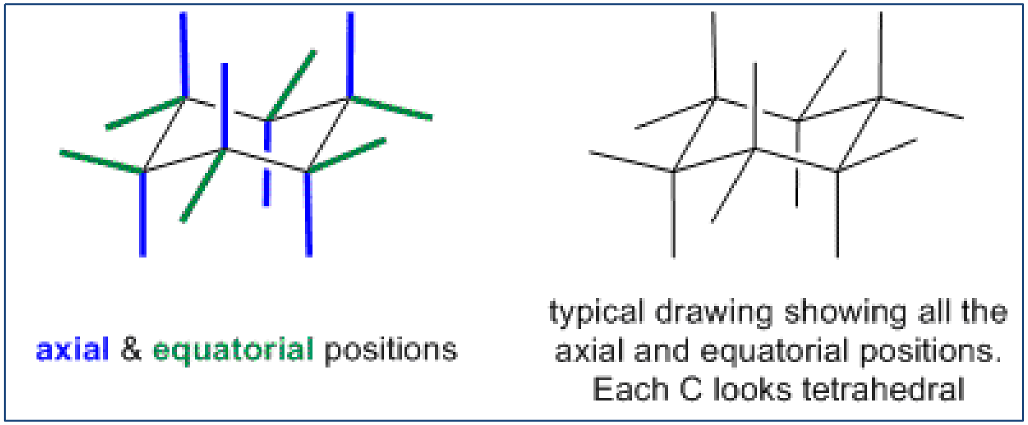


6.3 Putting it all together

1. Start by drawing your chair shape, making sure to watch your parallel lines!
2. Then add all the axial positions, alternating "up, down, up, etc"
3. Then all the equatorial position, this time starting with "down, up, down etc.

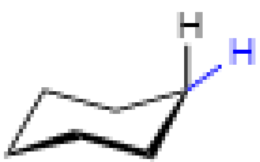


Now it is your turn! Draw out 2 chairs with all the axial and equatorial positions labeled!

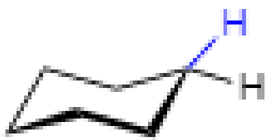


6.3 Mistakes to Avoid

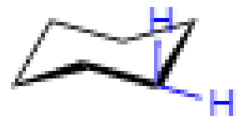
1. Make sure your outside lines are parallel.
2. Axial likes should be vertical!
3. Equatorial lines will be parallel with other lines in the structure of your chair.
4. EACH carbon will have an “up” and “down” position that alternates between axial and equatorial



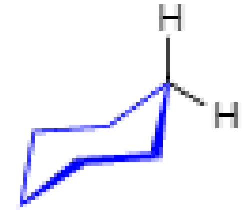
Incorrect.
Equatorial bond should be **down** and **out**.



Incorrect.
Axial bond should be **straight up**.

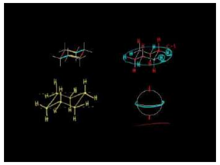


Incorrect.
Axial bond should be **straight down**, equatorial bond should be **up and out**.



Incorrect.
Ring should be tilted slightly.
YouTuber Leah4Sci draws them like this - it's technically ok, but try to avoid it!

Video tutorial for drawing/labeling chairs. Note: It also shows the flipped chair towards the end!



READ Pages 115-118 in the Klein Packet (Section 6.3)

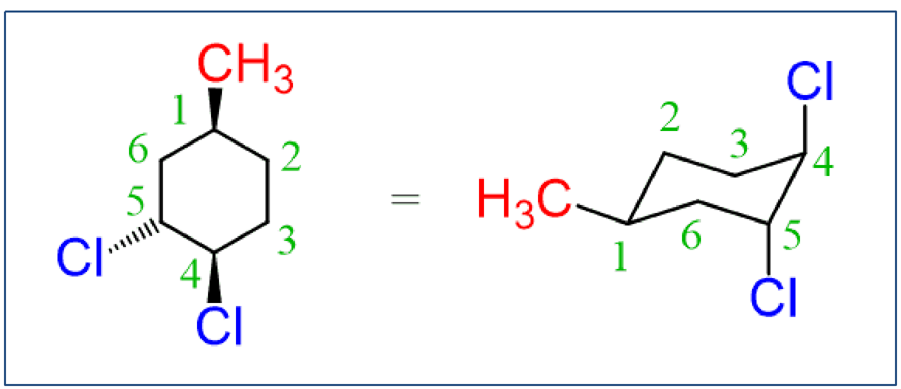
6.4 Placing Groups on the Chair

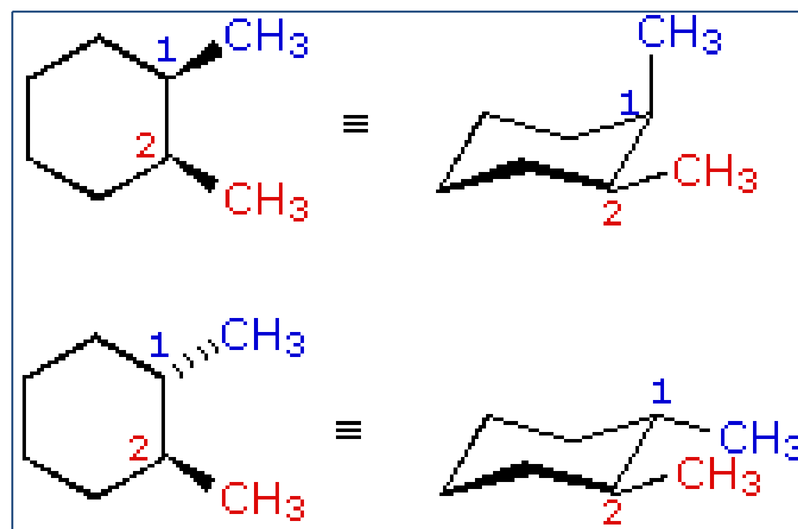
1. __________ are coming towards us on the paper, these will be in an "___" position.

2. _________ are going into the plane of the paper, these will be in a "_______" position

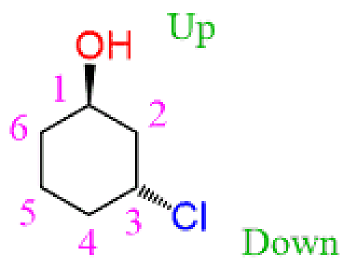
3. *You can actually start at any carbon*, but Mrs. H. likes to always reference the top carbon on the cyclohexane an the top right on the ring as carbon #1 and move clockwise. *(They aren't the same numbers as we use in naming - we could rotate this around!)*

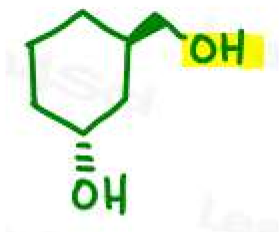
4. **You only need to show the axial & equatorial positions of the carbons that have "stuff" on them.**

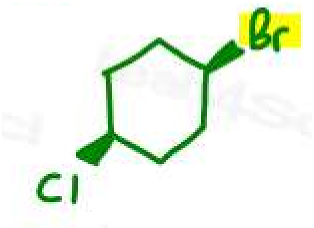




6.4 Practice Making a Cyclohexane into a Chair



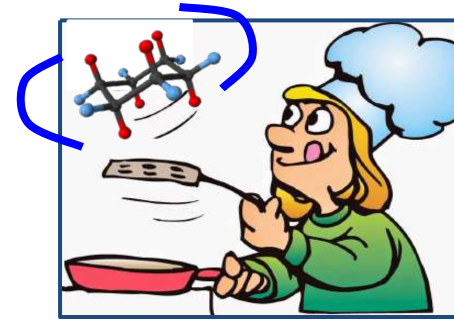




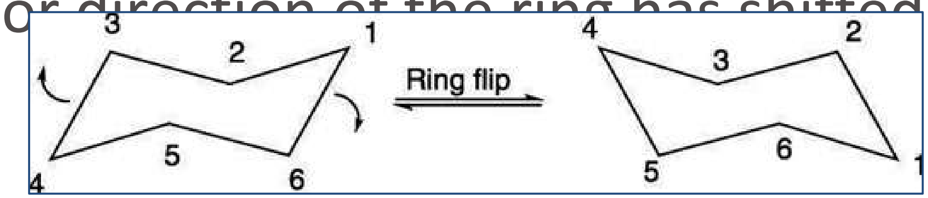
READ Pages 118-122 in the Klein Packet (Section 6.4) and complete **practice problems 6.15-6.21**

6.5 Ring Flipping

- Flipping a chair is <u>not</u> like flipping a pancake. Flipping a chair is the result of C-C single bonds rotating ONLY.



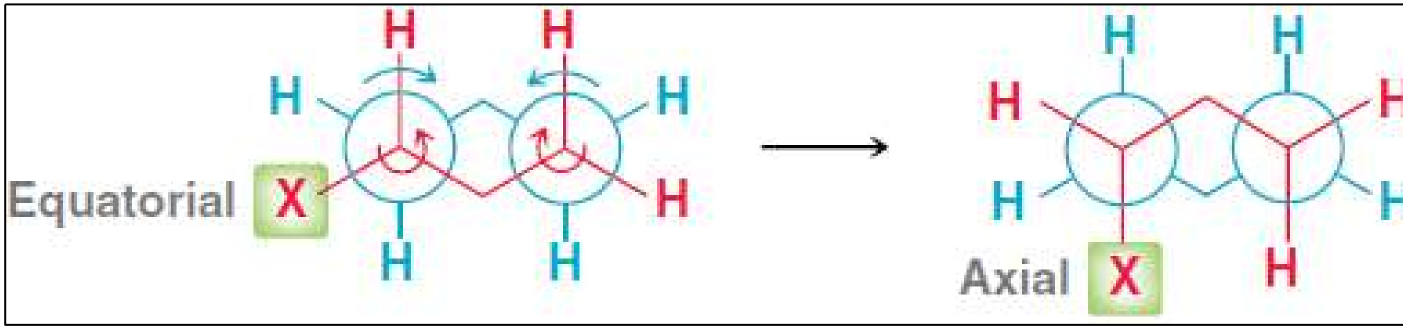
- It is actually more of a "shimmy" or "shift"
- Notice the slant or direction of the ring has shifted.



- Practice drawing 2 of the flipped (reversed) rings below!

6.5 More About Ring Flipping

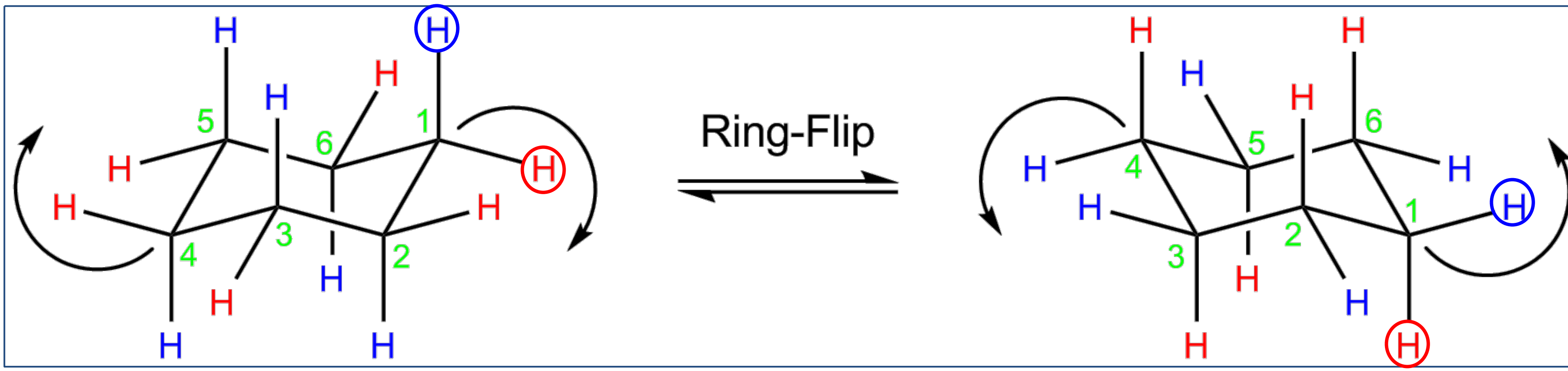
- The Newman projection below shows how flipping occurs ONLY through rotating bonds and how it will affect the axial or equatorial position of the substituent



- Such flipping is MUCH easier to see with a handheld model. Try it yourself! *(Make the substituents alternating colors of white and green)*
- *What happens when you flip the ring to your equatorial and axial positions?*
- *What about the up/down aspect?)*

6.5 Ring Flipping

- We have to learn the equatorial and axial positions of the flipped chair as well.
- **Notice that only the concept of axial/equatorial is switching. the “up/down” terminology stays the same!**

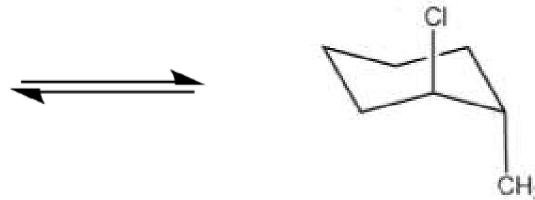


- *Practice drawing 2 of the flipped (reversed) rings below with all of the axial/equatorial positions drawn!*

6.5 Practice Doing a Ring Flip

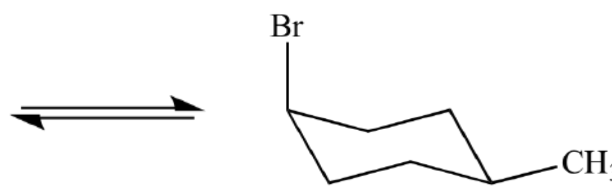
CLICK HERE for the answers!

1.



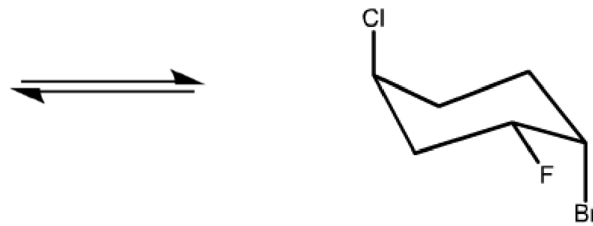
Work backwards!

2.



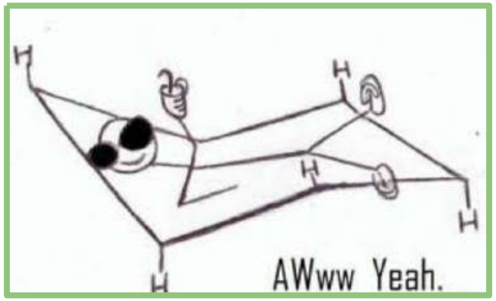
Work backwards!

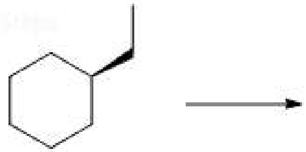
3.

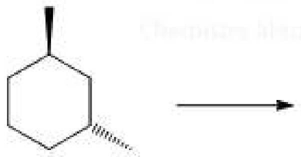


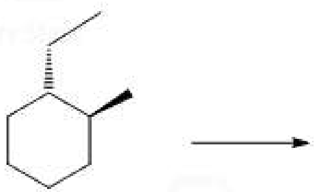
Work backwards!

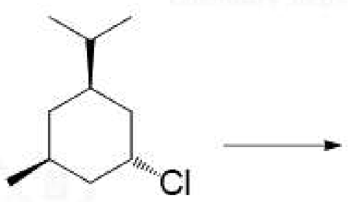
6.5 Practice Making Both Chairs

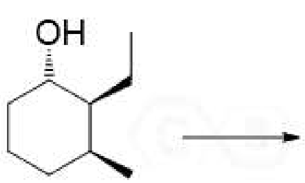


a) 

b) 

c) 

d) 

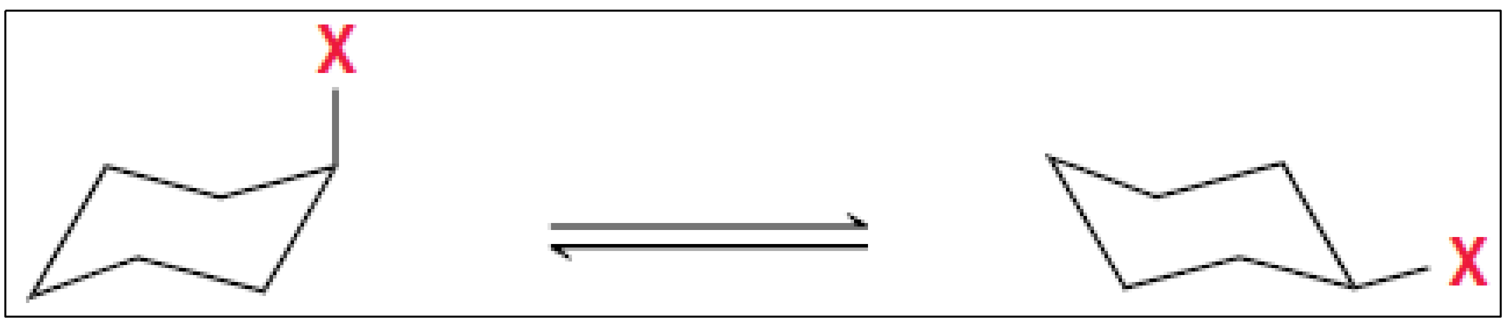
e) 

READ Pages 118-123 in the Klein Packet (Section 6.5) and complete **practice problems 6.22-6.36**

6.6 Comparing the Stability of Chairs

- The vast majority of cyclohexane molecules will exist in the chair conformation at any given moment. WHY?

- When energy (45 kJ/mol) is available, it can ***flip*** from one chair form to another.
  - Why do you think energy is needed? *(Think of spontaneous things in nature!)*
  - *Which "position" (axial or equatorial) do you think is more "comfortable" for the substituent?*



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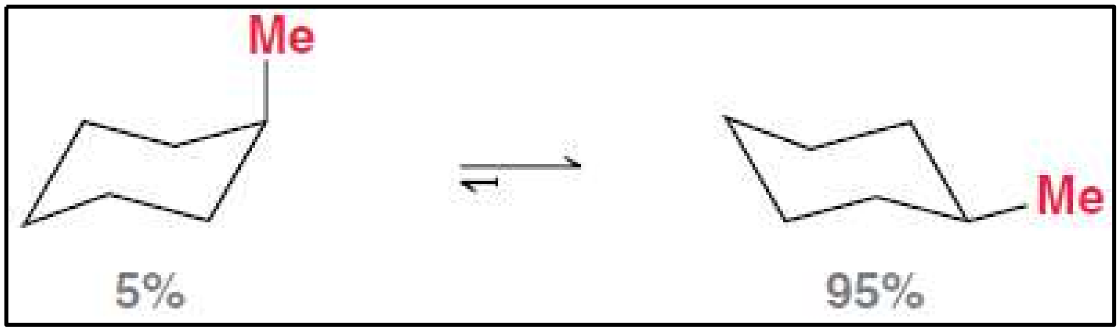
6.6 Comparing the Stability of Chairs

- **If both versions of the CHAIR were equally stable, you would have a 50/50 mixture of axial/equatorial**
- Consider methylcyclohexane



- Why does the equatorial chair dominate the equilibrium?
- Does the axial substituent cause additional angle or torsional strain?

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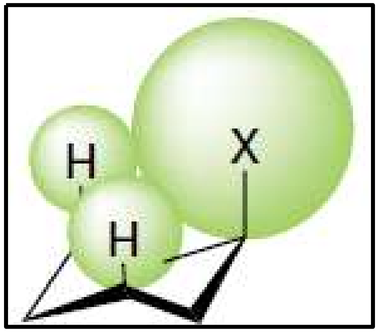
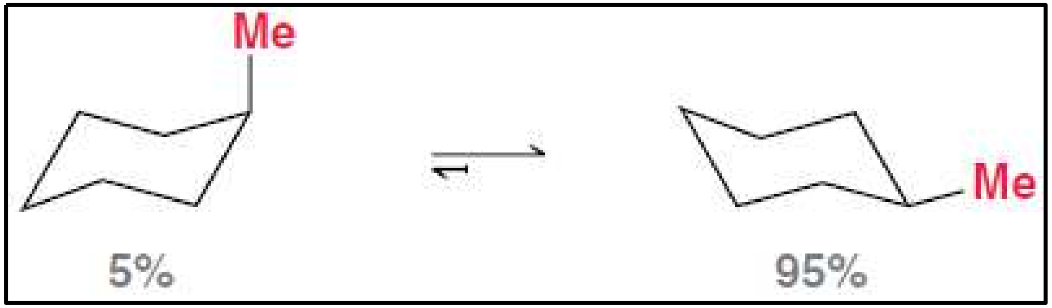
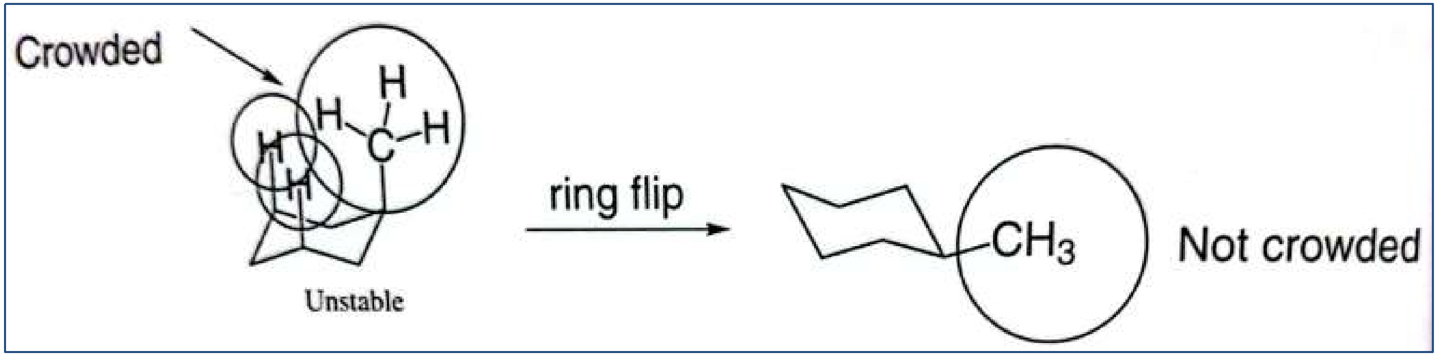
6.6 Comparing the Stability of Chairs

- The axial substituent causes additional steric strain





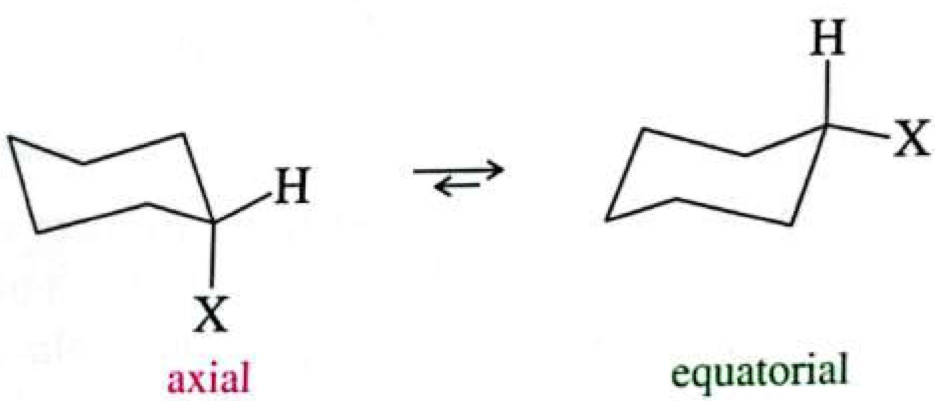
- Such steric crowding is called "**diaxial strain**", specifically, the molecule above has "1,3-diaxial strain". WHY?
  - This "strain" can also be called "**steric hindrance**"
  - you may have to "flip" the ring to see which conformation will be present the most.



6.6 Comparing the Stability of Chairs

The effect of steric hindrance can be calculated. We won't do calculations with these values, but this table shows which atoms/groups experience higher levels of hindrance. You will see on the following slides how to use these to determine stability of chairs.

TABLE 3-6 Energy Differences Between the Axial and Equatorial Conformations of Monosubstituted Cyclohexanes

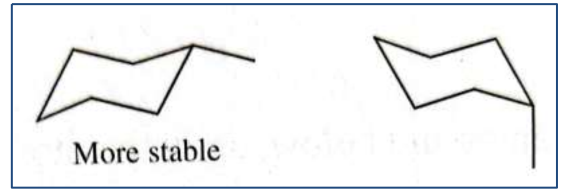


X	ΔG (axial–equatorial) (kJ/mol)
—F	0.8
—CN	0.8
—Cl	2.1
—Br	2.5
—OH	4.1
—COOH	5.9
—CH_3	7.6
—CH_2CH_3	7.9
—$CH(CH_3)_2$	8.8
—$C(CH_3)_3$	23

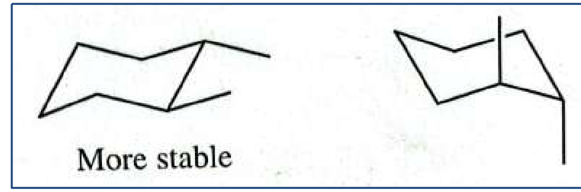
Increasing hindrance in the axial position

6.6 Comparing the Stability of Chairs

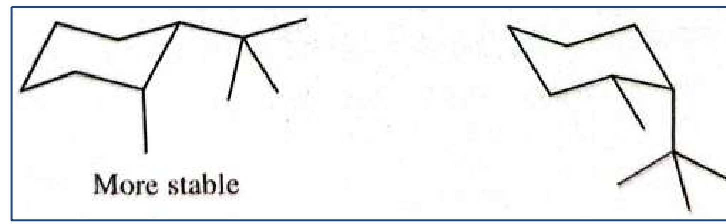
- If you have one group on the ring, the more stable chair will have it in the equatorial position.



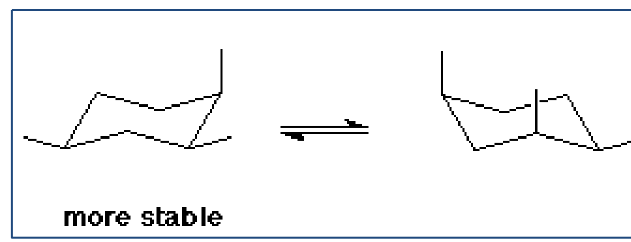
- If you have 2 groups on the ring, its most stable when both groups are in the equatorial position…



  - **If both can't be in the equatorial position**, the larger of the two groups will be more stable in the equatorial position.



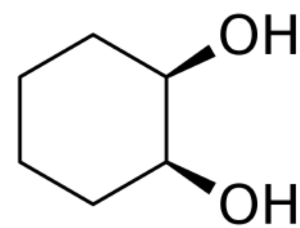
- If you have *more than 2 groups,* use the same logic we used above!



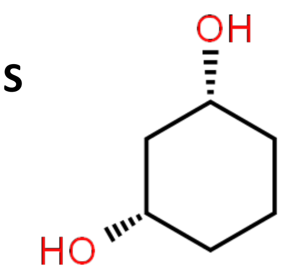
PRACTICE: Go back to where you drew out both chairs on the previous slides for section 6.5 (#1-5 and a-e), **circle the more stable chairs**. If there is a tie, explain why! **Then, read Klein packet pages 129-133 (section 6.6) and answer questions 6.38-6.45.**

6.7 Don't be Confused by Nomenclature

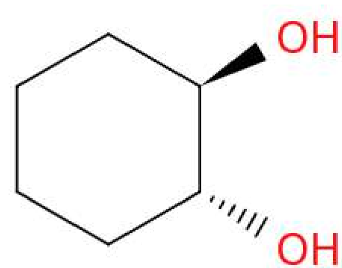
- Some nomenclature can be confusing. We will see terms like "cis and trans" when we don't have double bonds.
- When we have 2 groups **both** "up" or **both** "down", we say they are *cis* to each other.



BOTH are CIS

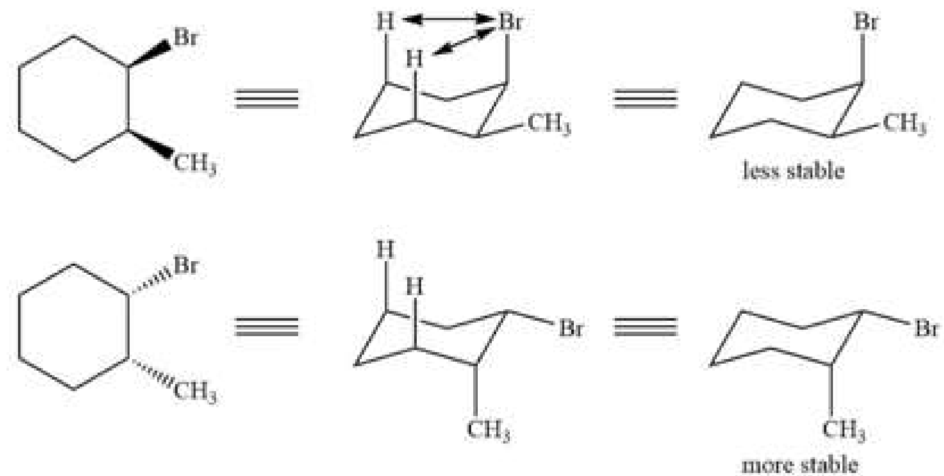


- When we have 2 groups and **one** is "up" and the **other** "down", we say they are *trans* to each other.
  - Axial/equatorial does not matter here!
  - Remember -ane- means all single bonds

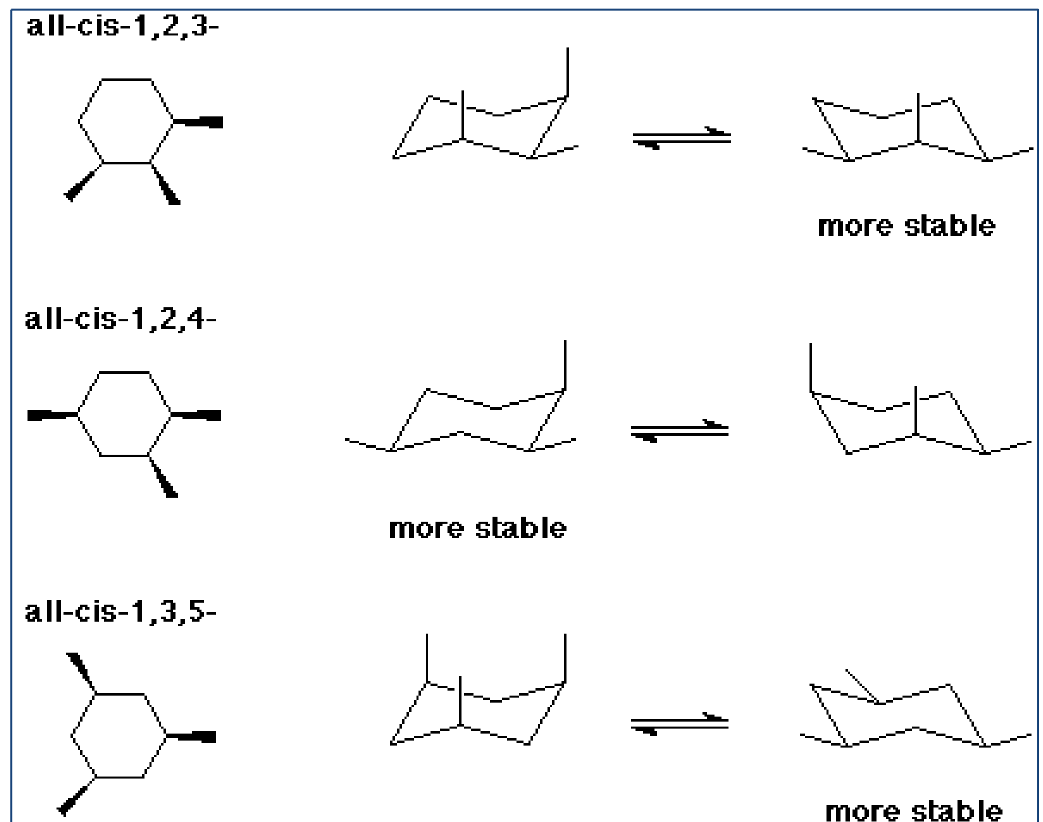


6.7 Don't be Confused by Nomenclature

- Cis and Trans can be used for cyclohexanes that have more than just 2 groups



  - In these examples the groups are all cis to each othe: they would all be on wedges *(or dashes - not shown)*



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6.7 Don't be Confused by Nomenclature Practice

1. Determine if the cis or trans conformation of para-dibromocyclohexane would be more stable. *(Hint: you will want to draw each possibility out, don't forget about the flipped rings! Once you "get it" you won't have to do as much work!)*

READ Page 133 (section 6.7) in your Klein Packet

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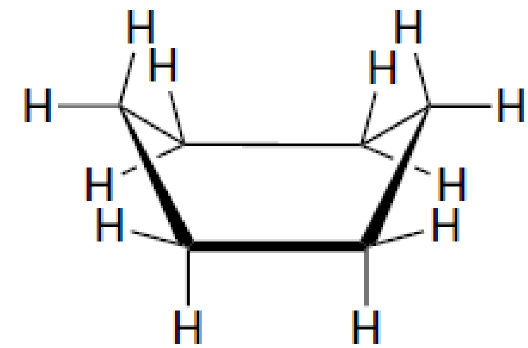
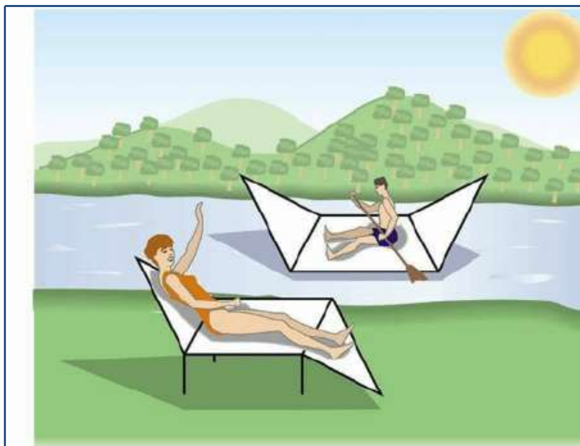
More types of Conformations for Cyclohexanes

- Other conformations of hexane exist but are a bit less stable. Consider **THE BOAT**



1. No angle strain - angles are 109.5°
2. Torsional strain.
   - Use a molecular model to identify all four pairs of eclipsing C-H bonds
   - Draw a Newman projection that illustrates the torsional strain
3. Steric strain – flagpole interactions. WHERE?

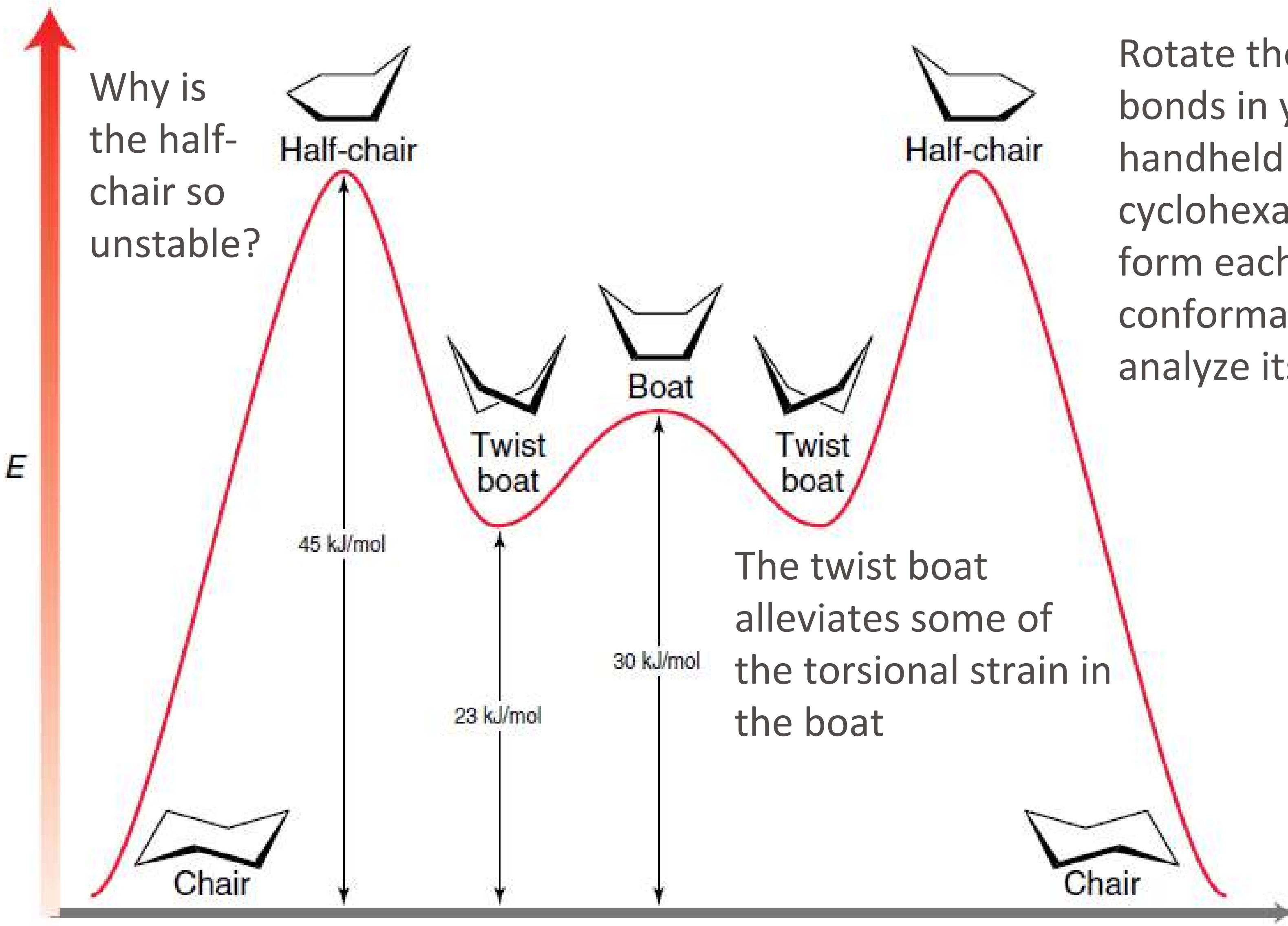
- Why is this conformation called the BOAT?
- You can create a cyclohexane model and create the conformations.



I bet that boat will sink . It is less stable than chair conformation 😂

Cyclohexane Conformations

Why is the half-chair so unstable?



Rotate the C-C single bonds in your handheld cyclohexane model to form each of the conformations and analyze its energy

The twist boat alleviates some of the torsional strain in the boat

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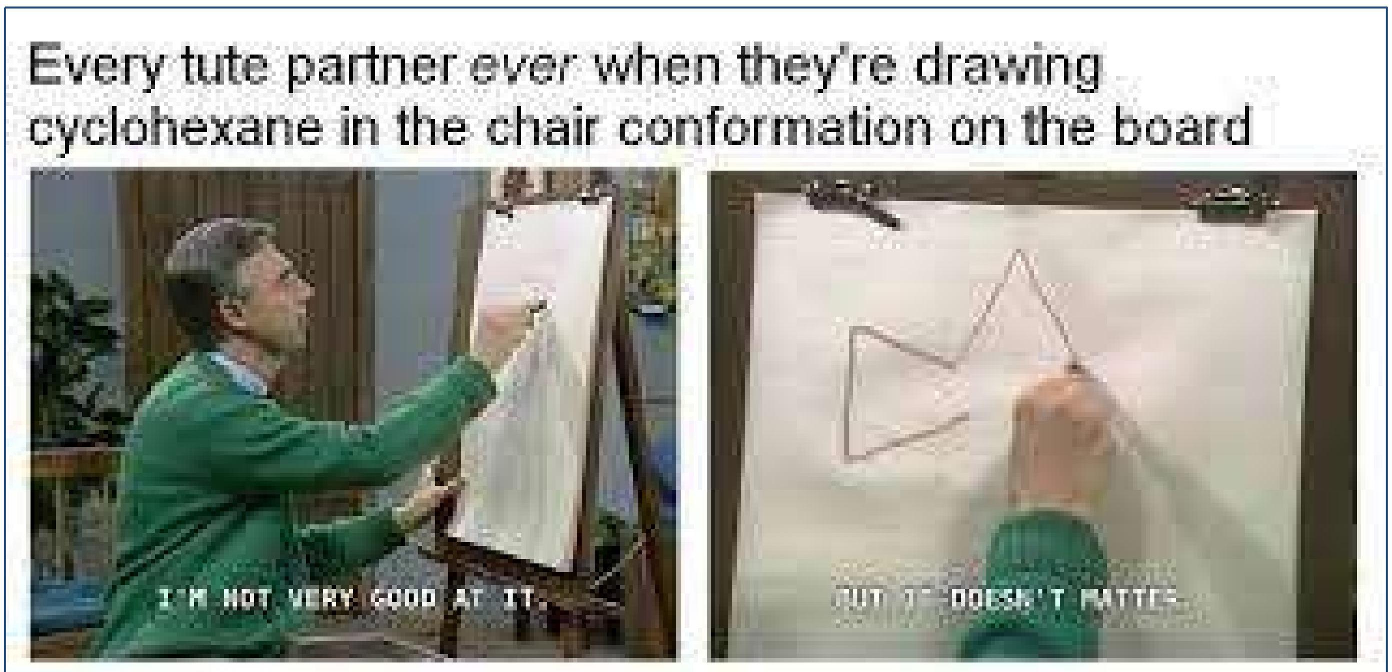
Because we love nerdy memes!



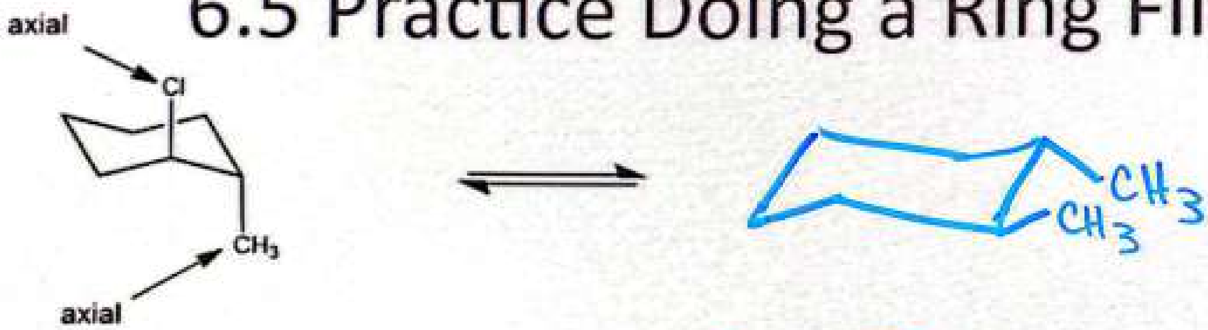
There are extra practice videos embedded in the google slide notes posted on google classroom!

END OF STUDENT SLIDES

SOLUTIONS TO FOLLOW

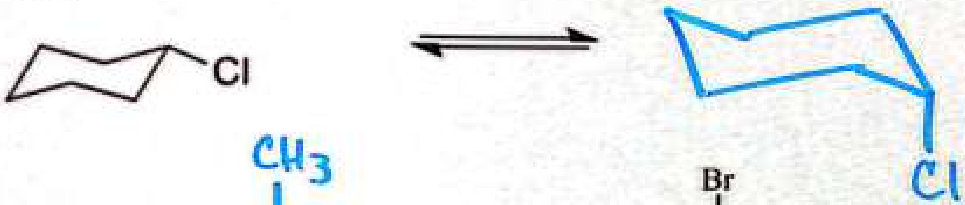
6.5 Practice Doing a Ring Flip

2.

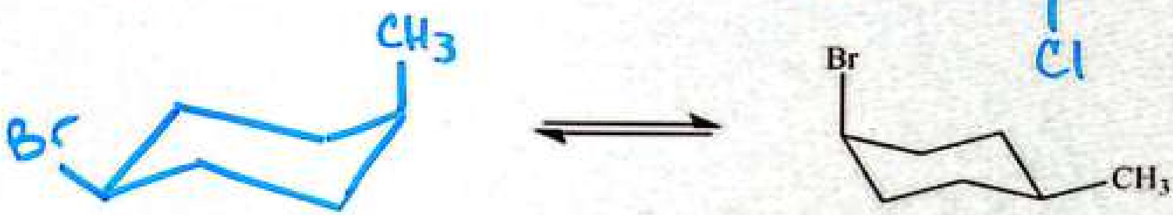


✱ Work Backwards!

1.

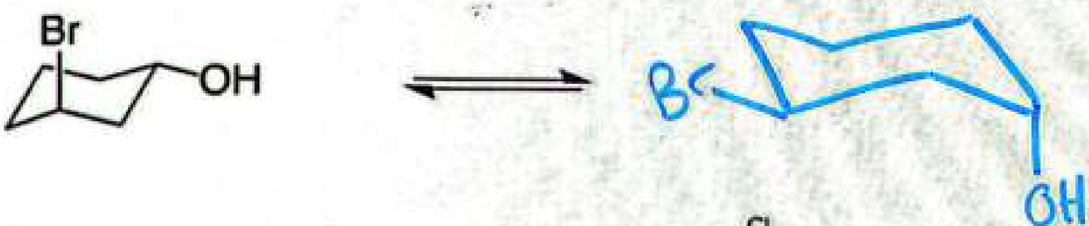


4.

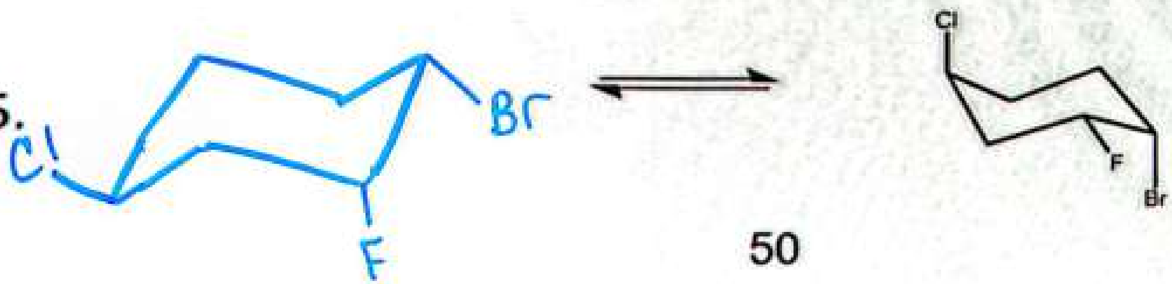


Work backwards!

3.

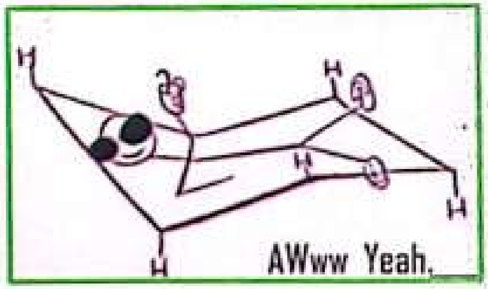


5.



Work backwards!

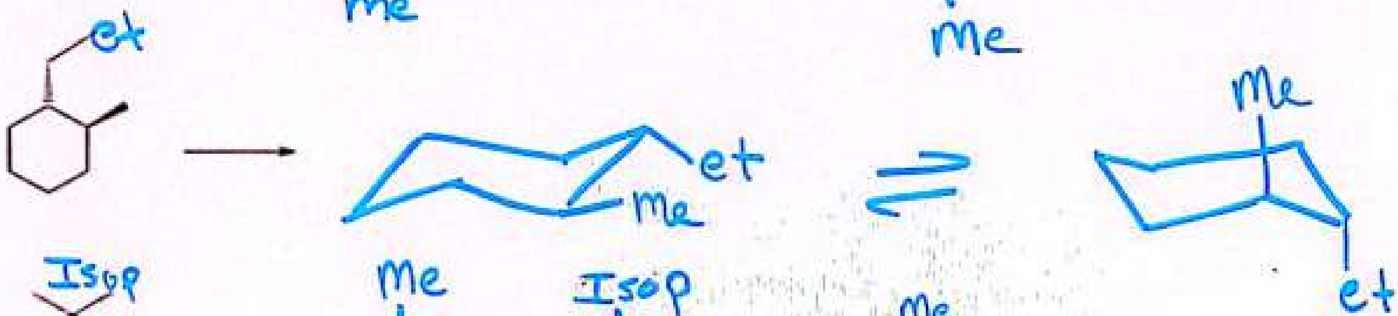
6.5 Practice Making Both Chairs



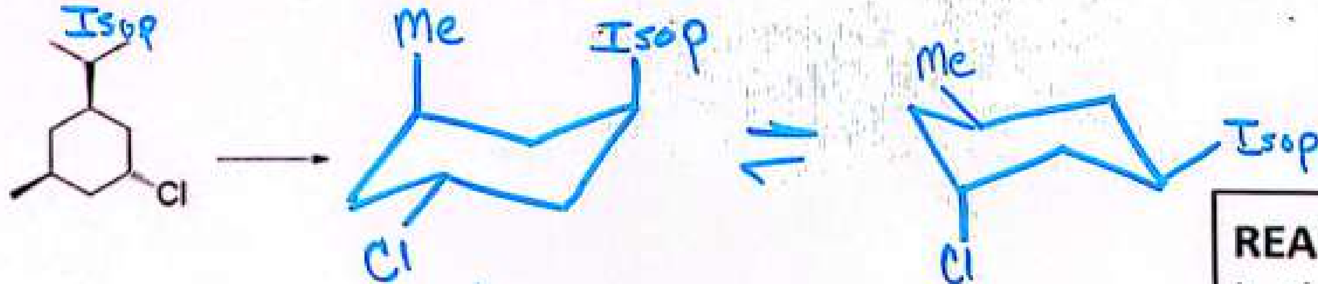
a)

b)

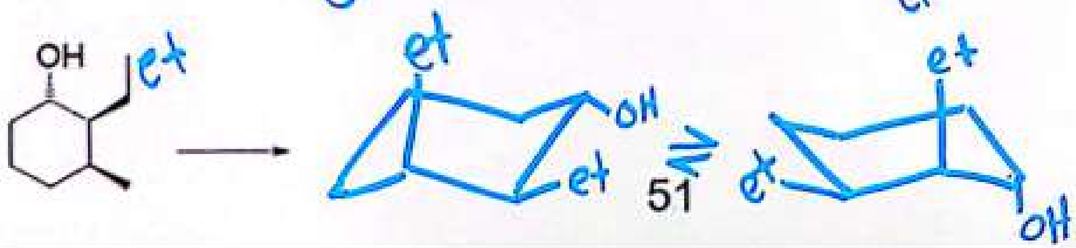
c)



d)



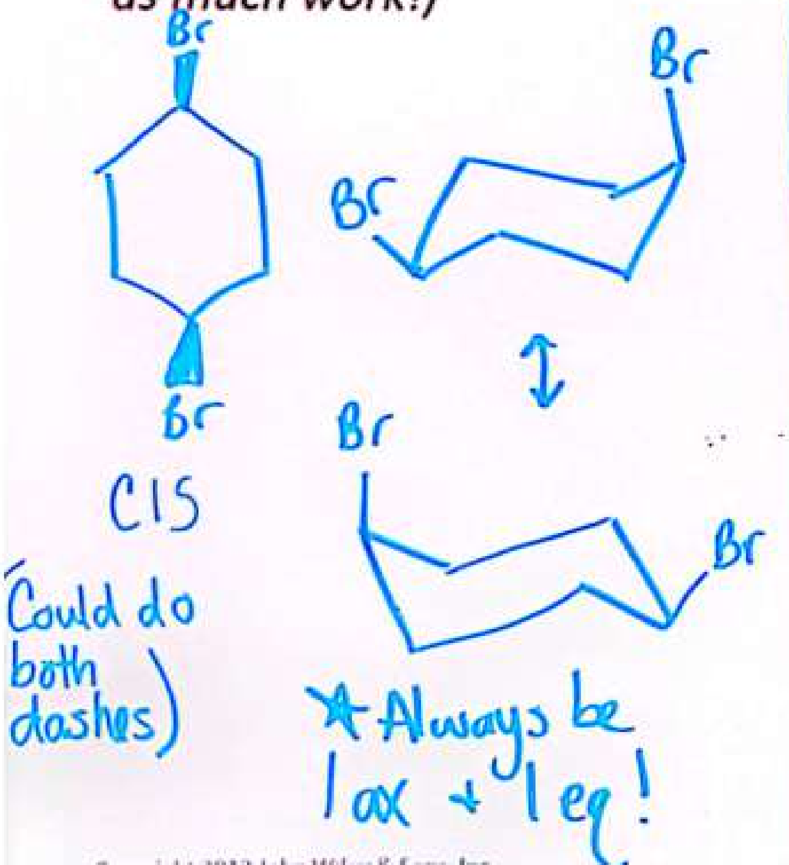
e)

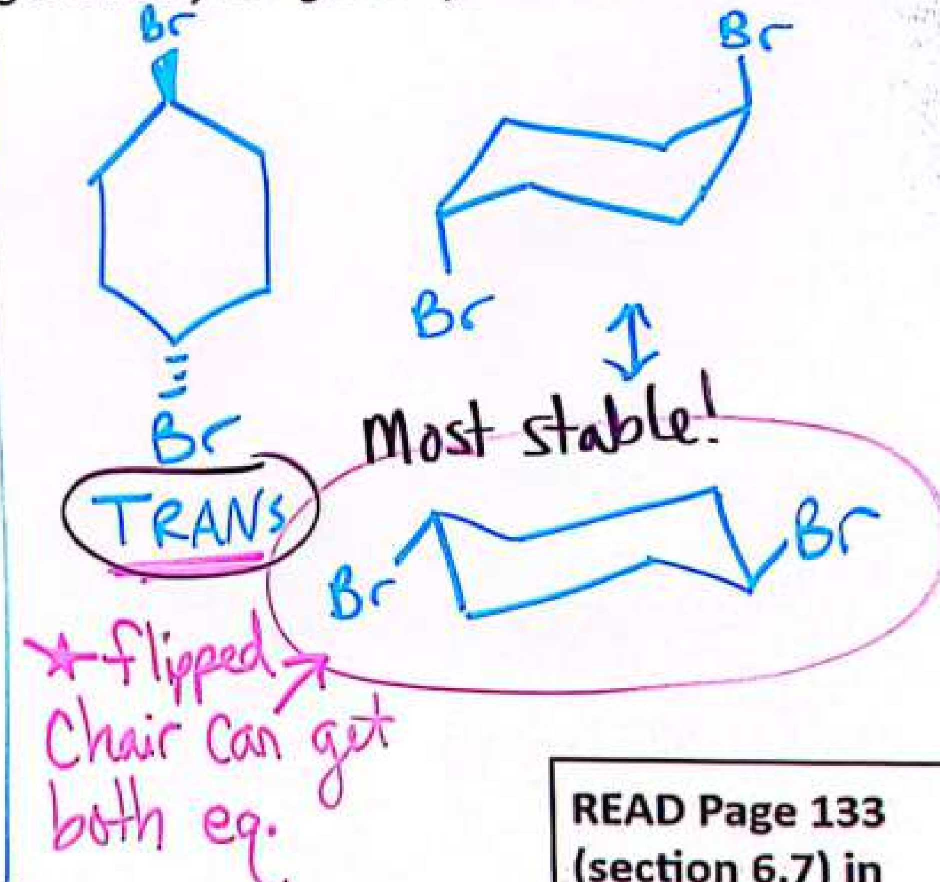


READ Pages 118-123 in the Klein Packet (Section 6.5) and complete **practice problems 6.22-6.36**

6.7 Don’t be Confused by Nomenclature Practice

1. Determine if the cis or trans conformation of para-dibromocyclohexane would be more stable. *(Hint: you will want to draw each possibility out, don’t forget about the flipped rings! Once you “get it” you won’t have to do as much work!)*





READ Page 133 (section 6.7) in your Klein Packet

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