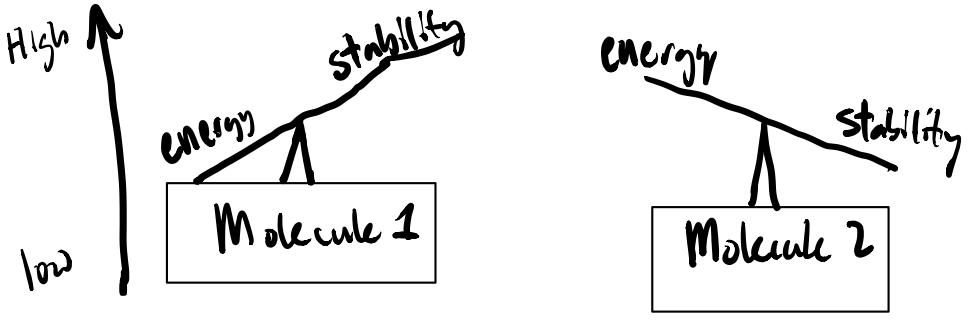
MTW

Today: Strain
Stability
Newman Projections
Chairs
Stereochem

Energy & Stability are interrelated
↳ influenced by strain } 3 Types
1) Torsional
2) Steric (Non-Bonded)
3) Ring Strain (Angle Strain)

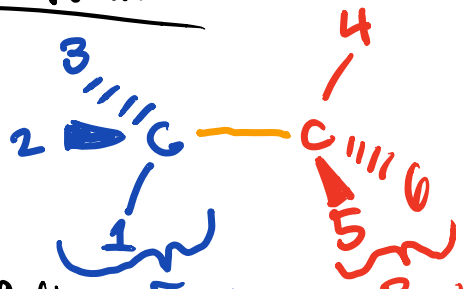


- More Strain → Higher in Energy & Less Stable
- Strain is influenced by Conformation
  ↳ 3D arrangement of atoms in a molecule resulting from rotations around bonds

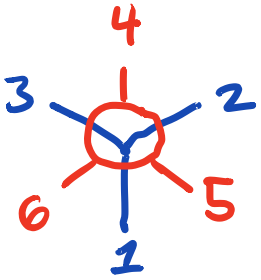
One convenient way to look at conformation (in turn stability & strain) is w/ a Newman Projection, where we look down/along a specific bond.

Newman Projection Format

tells us where we look from



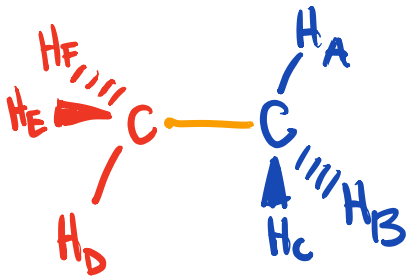
define Front Atoms / Back Atoms

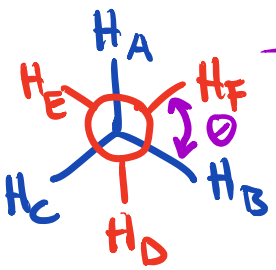


- C atom in front (closer to eye) drawn as Y

- C atom in back drawn as big circle

Staggered Ethane (CH_3-CH_3)



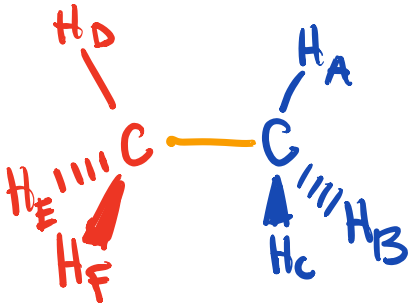


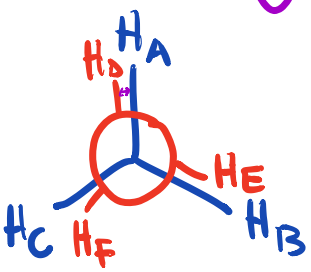
Staggered
$\theta = 60°$
↳ No Torsional Strain

H_A & H_D are "anti" (opposite)

If $\theta \neq 60°$, there is some torsional strain

Eclipsed Ethane





Eclipsed
$\theta = 0°$ (zero)
↓
Torsional Strain

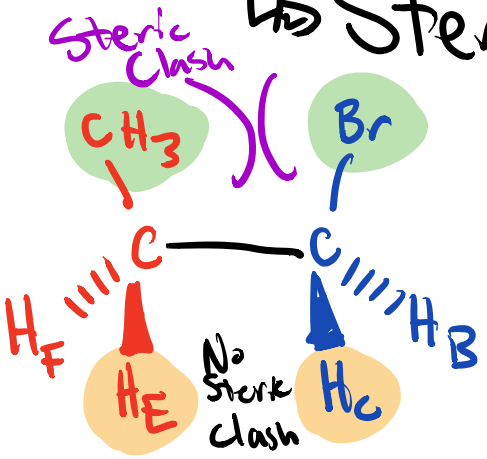
H atoms are small, so they never hit each other, even when eclipsed

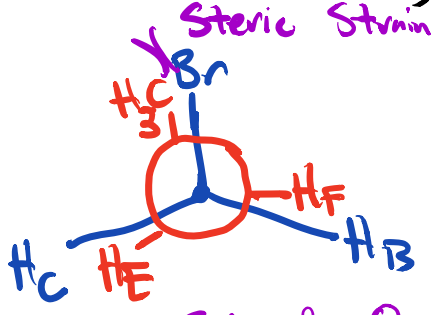
↳ H_A & H_D above don't "clash" in space

↳ No Steric Strain between 2 H atoms!

But Bigger atoms or groups (e.g. Cl, Br, $-CH_3$) can "clash" or hit each other in space

↳ Steric Strain (Non-Bonded Strain)



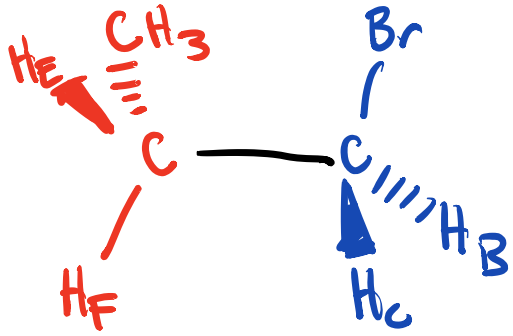


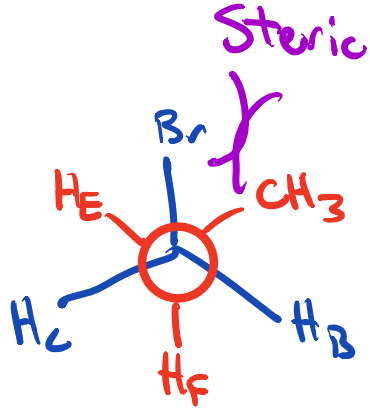
Eclipsed = $\theta = 0°$ → Strain also

Torsional

Do these two atoms hit each other? No.

Do these two "groups" hit each other? Yes!

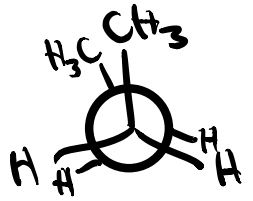




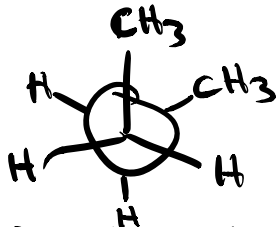
Staggered ($\theta = 60°$)

No Torsional Strain

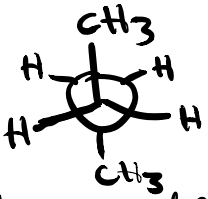
But Steric Strain still



Eclipsed Butane



Gauche Butane

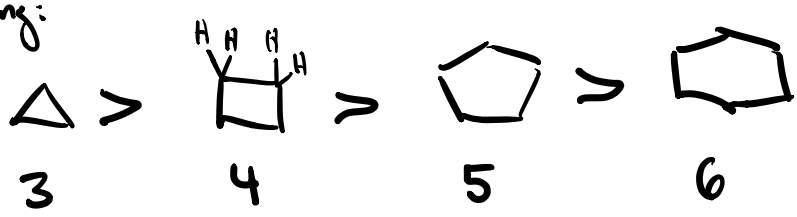


Anti-Staggered Butane

	Eclipsed Butane	Gauche Butane	Anti-Staggered Butane
Torsional Strain:	Yes	No	NO
Steric Strain:	Yes!	Yes	NO

Ring/Angle Strain → in a ring

atoms in ring:



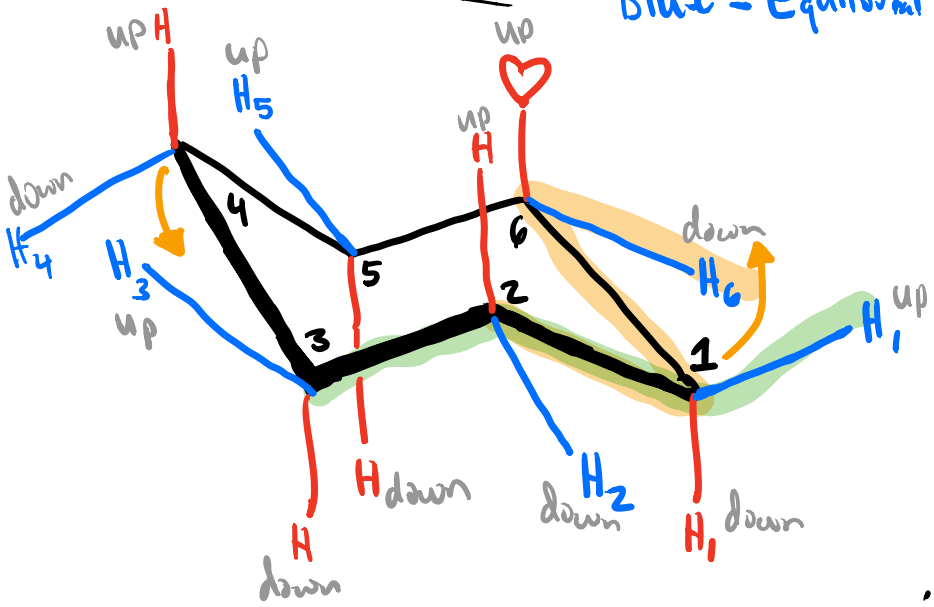
Cyclohexane ⇓ No ring strain

← Increasing Ring Strain

* Break until 1:19pm CST (5 min)

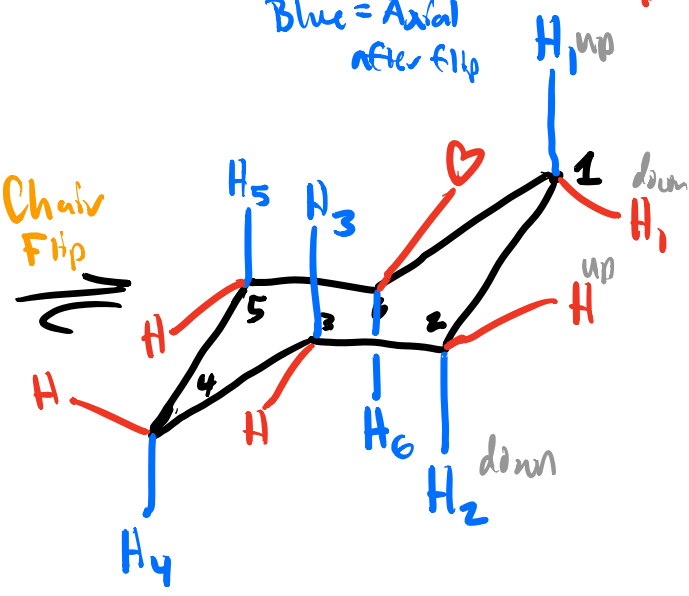
Chair Conformation

Red = Axial
Blue = Equitorial



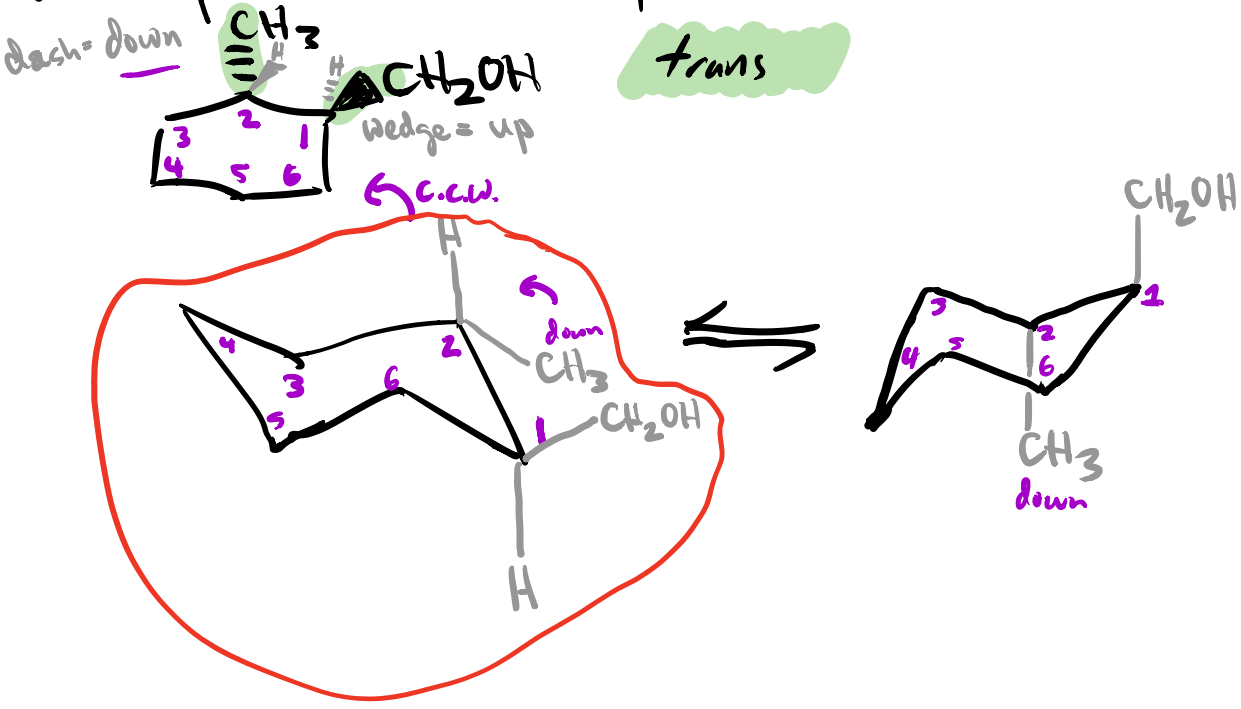
Red = Equit. after Chair flip
Blue = Axial after flip

Chair Flip ⇌

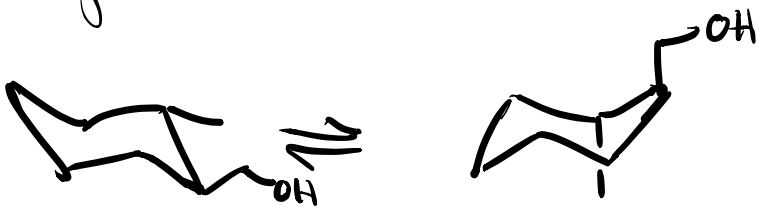


Larger groups prefer to be equitorial

Draw 2 Chair Conf. for the following & circle which predominates at equilibrium:



Another way to draw the above:



Stereochemistry

Isomer → same chemical formula

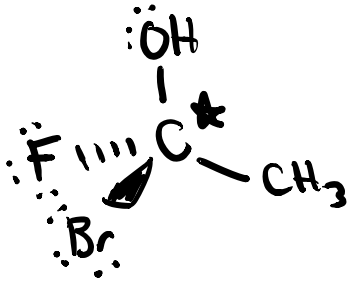
$C_4H_{10}O$

Constitutional Isomers → same molecular formula but different connectivity

$C_4H_{10}O$ 

Stereoisomers → same constitutional isomers, same bond connectivity but different arrangement of groups in 3D space

C_2H_4OFBr



Chiral Center: 4 different groups around a tetrahedral atom

Chirality: Phenomenon for objects that are not superimposable on their mirror image.

Enantiomers = non-superimposable mirror images

Diastereomers = Stereoisomers that aren't enantiomers
↳ need at least 2 chiral centers

Meso Compound = 2 chiral centers, but itself is not a chiral object
Each chiral center has the same 4 groups

Assigning Chirality → assigning R/S

↳ playing card game 1st point of difference

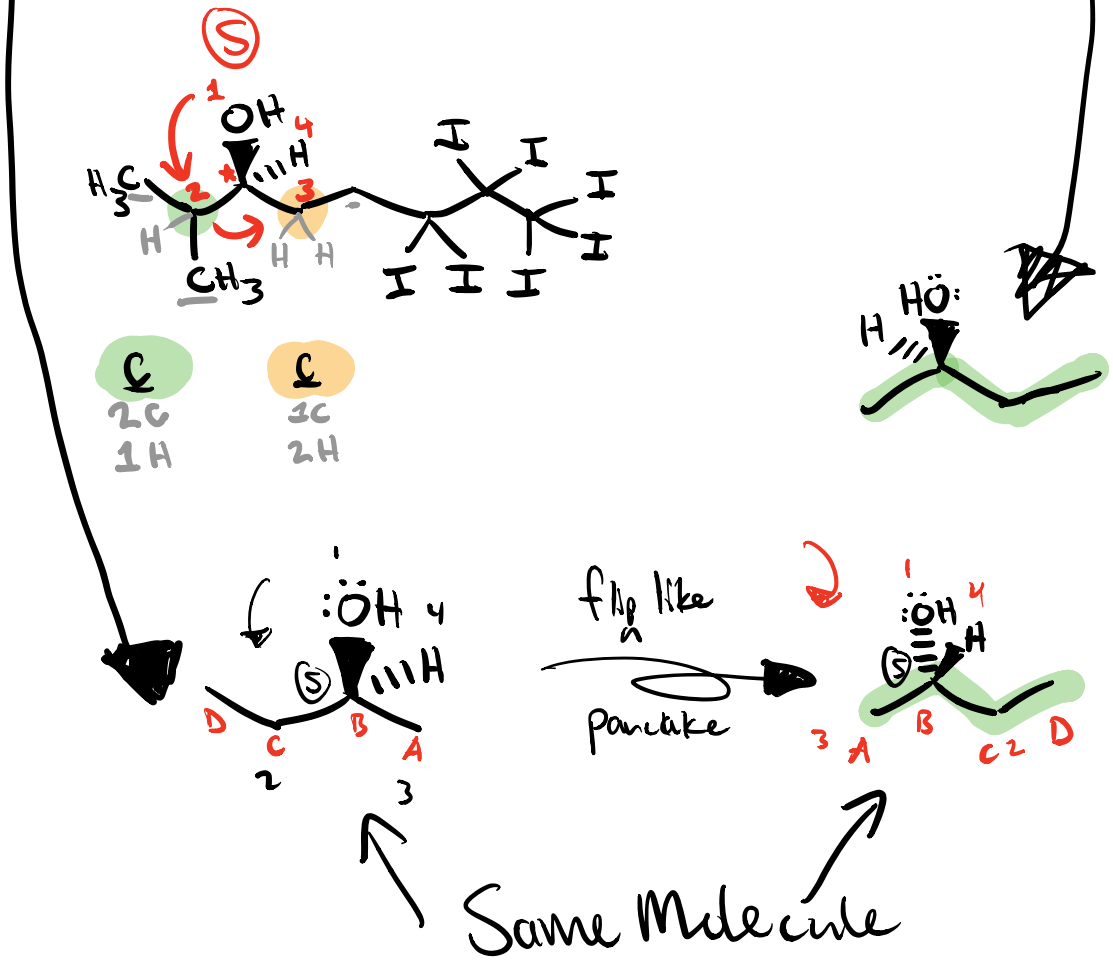
1. When lowest priority group is in back (≡)

Clockwise — R

CounterClockwise — S

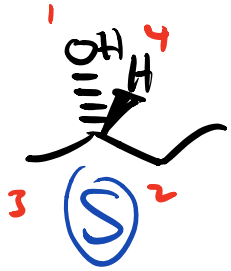
The mirror image of R is S.

The mirror image of S is R.

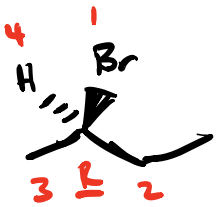


[2] lowest priority group is in front

"looks R, but lowest priority is in front, so its S"



Aside:



Wedge on Left vs. Right

⇓

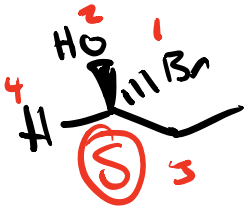
No difference in R/S

⇓

Same molecule

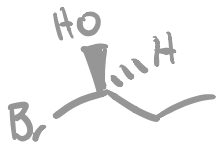
★ If you switch any 2 groups → You get the enantiomer! ★

[3] H-atom in plane of paper (lowest priority group)

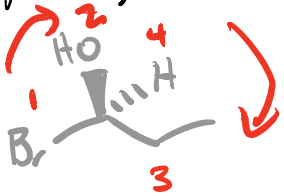


↔ S when looking down bond.

① If H/lowest priority group is in plane of paper
↳ switch H w/ group on dash (group in back)

① 

② Then assign R/S for this "swapped" molecule

② 

R

③ The actual chirality of the molecule you started with is the opposite (Because of ★ rule above)

③ S

* rotate a bond

* flip like pancake

* Turn

All the same molecule

⇓

Flips / Rotations / turns don't change it