MTW4 9-19

Monday, September 19, 2022 3:26 PM

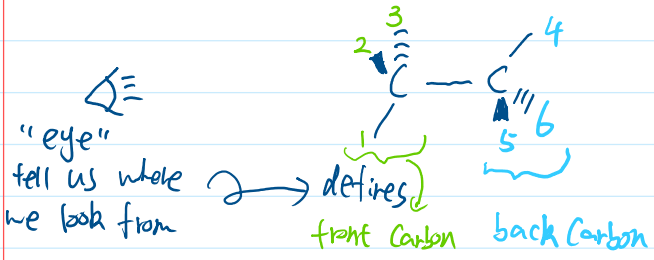
Today: . strain and stability
- Newman Projection
- Chairs
- Stereochemistry

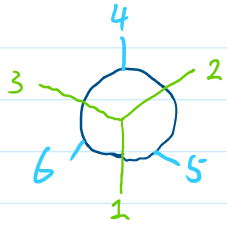
Energy and stability are interrelated
↳ influenced by strain { 3 Types
1) Torsional
2) Steric (non-Bonded)
3) Angle strain (ring strain)


- more strain → Higher in energy and 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 and strain) is w/ Newman Projection, where we look down/along a specific bond.

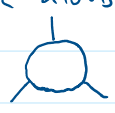
Newman Projection Format



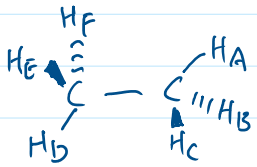




- C atoms in front (closer to a eye) drawn Y

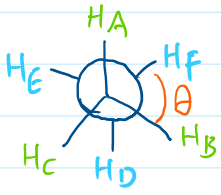
- C atoms in the back:



Staggered Ethane ($CH_3-CH_3$)

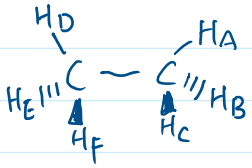



⇒ ($H_A$, $H_D$ are "anti")
(pointy opposite)

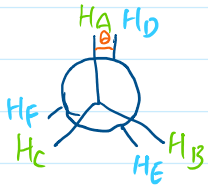



Staggered
$\theta = 60°$
↳ No Torsional strain
If $\theta \neq 60°$, there is torsional strain

## Eclipsed Ethane



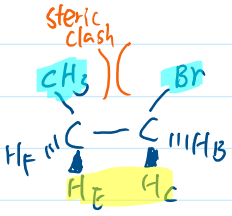

⇒



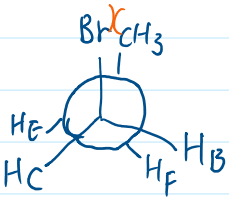

Eclipsed
$\theta = 0°$
↓
Torsional strain

H atoms are small, so they never hit each other, even when eclipsed
↳ $H_A$ and $H_D$ above don't "clash" in space
(NO steric strain w/ 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)




⇒
These groups hit each other
These groups do NOT hit each other

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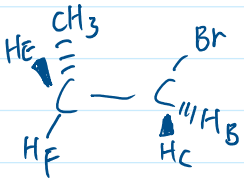
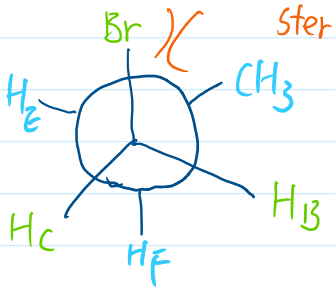


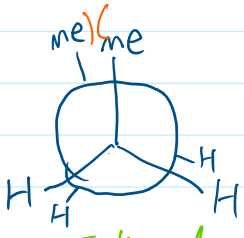

⇒



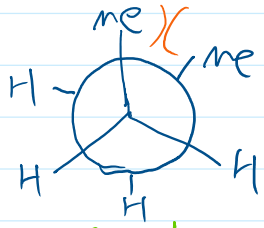

Gauche

Staggered ($\theta = 60°$)
No Torsional Strain

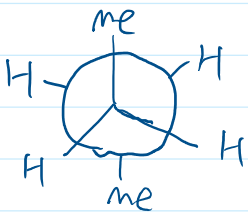
Staggered ($\theta = 60°$)
No Torsional Strain
But Steric Strain Still




Eclipsed




Gauche

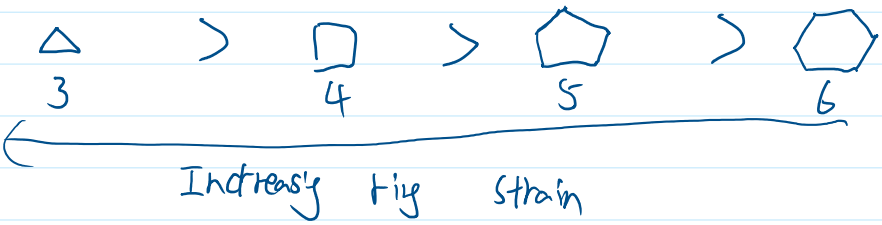



Anti-staggered

| | Eclipsed | Gauche | Anti-staggered |
|---|---|---|---|
| Torsional: | Y | N | N |
| Steric: | Y | Y | N |

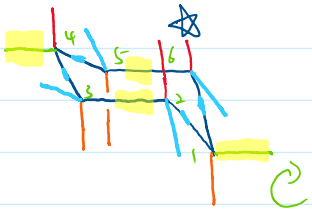
Angle/ring Strain: In a ring

# atoms in rings

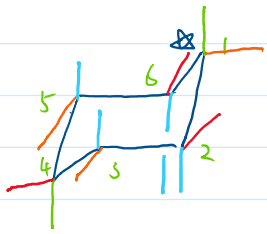



Cyclohexane ↓ No Angle Strain

Chair Conformation:



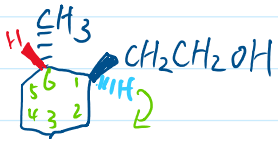

Chair Flip

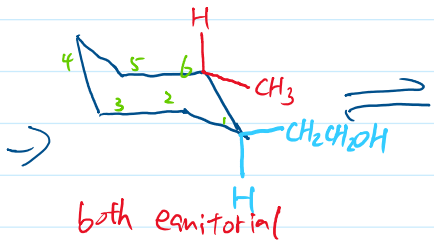



Chair Flip will NOT interconvert a "pancake" flip axial and equitorial groups

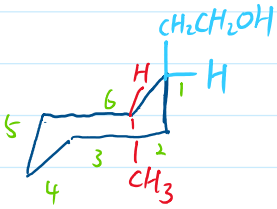
Larger groups prefer equitorial to release Steric Strain

e.g.: Draw 2 chair conformation for the following molecule and determine which one is favored at e.q.



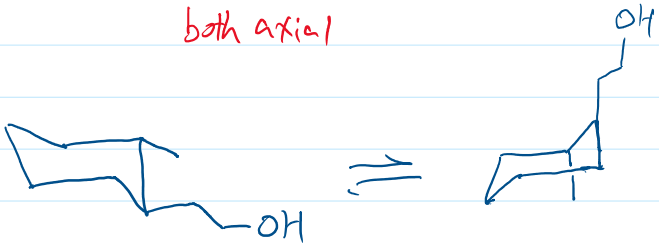




both equitorial




both axial

Left one is more stable




Back in 7:25 pm

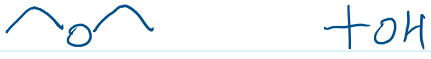
## Stereochemistry

Isomer → same chemical formula

$C_4H_{10}O$

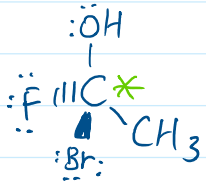
Constitutional Isomer → same molecular formula, but different connectivity

$C_4H_{10}O$




Stereo isomers → same constitutional isomer, 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 object that are not superimposable on their mirror image

Enantiomers: non-superimposable mirror images

Diastereomer: stereoisomer that aren't enantiomers
↳ at least have 2 chiral centers

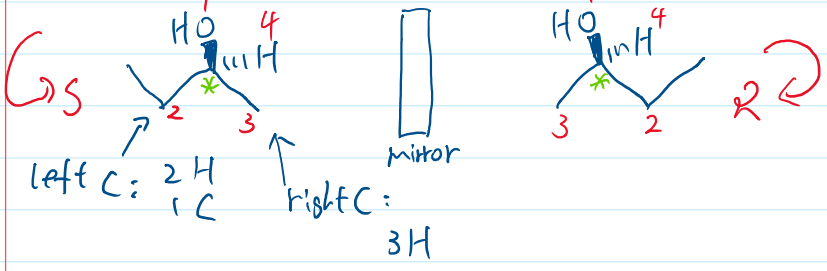
meso compound: 2 chiral centers, but itself is not a chiral molecule
Each chiral center has the same 4 groups.

Assigning chirality → assign R/S

↳ "playing card game", 1st point of difference

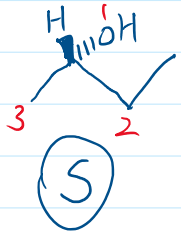
[1] when the lowest priority group is in back (≡)

clockwise R  counter clock wise S




The mirror image of S is R, the mirror image of R is S

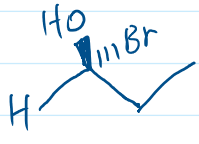
[2] lowest priority group is in front (▮)
"looks R, but lowest priority is in front, so it's S"



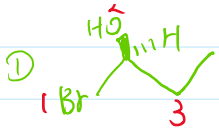

"R" looks R, but it's S

[3] lowest priority group is in the plane ("|" solid line)

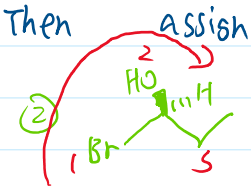
If we switch any 2 groups → we get the enantiomer!




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



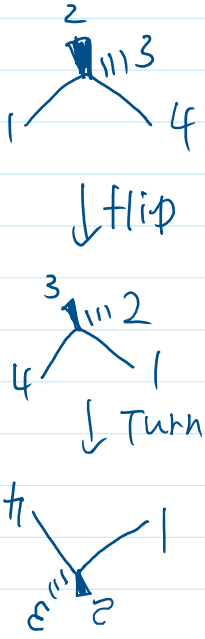

② Then assign R/S for the "swapped" molecule




R

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

③ S



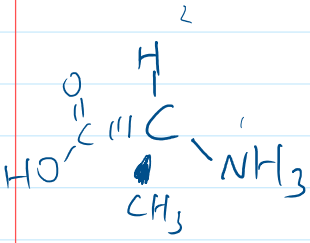


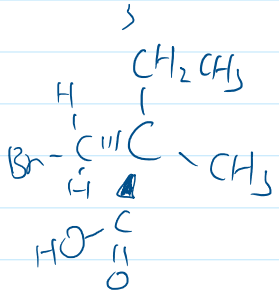
All the same molecule

↓

Flips / rotations / turns

do NOT change chirality

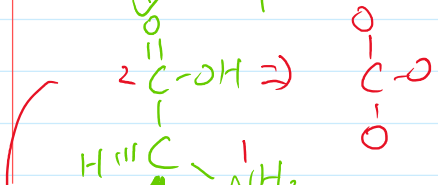


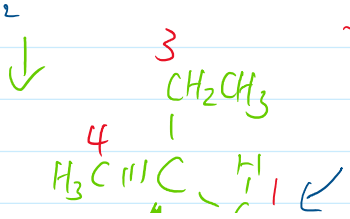




R

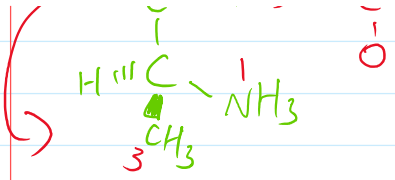
"Swap"

S

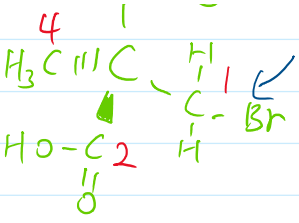



C : 1 Br



looks S, actual R



C : 1 Br
2 H

C : 3 O-atom

looks R, actual S