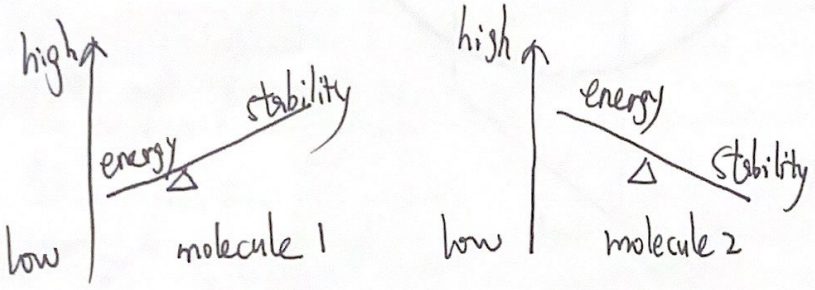
MTW

Topic: Strain and stability

Newman projections

Chairs

Stereochemistry

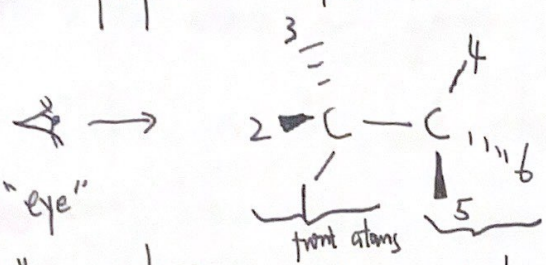


Energy and stability are interrelated.
↳ influenced by strain { 3 types
1) torsional
2) steric (non-bonded)
3) Angle strain (Ring strain)

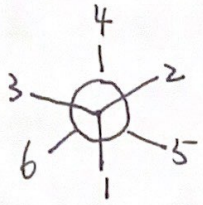
- more strain → higher in energy, less stable
- strain is influenced by conformation
↳ 3D arrangement of atoms in a molecule resulting from rotation around bonds.

One convinient way to look at conformation (in turn stability and strain) is with a Newman projection, where we look down/along a specific bond.

an projection Format



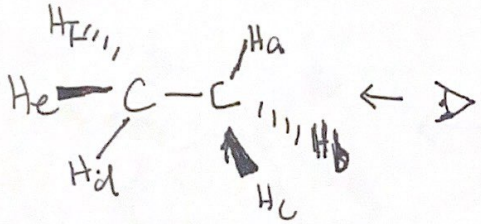
tells us where we look from → define

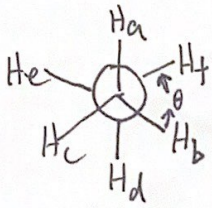


{ C atom in front (closer to eye) drawn as Y

C atom in back drawn as big circle

Staggered Ethane (CH_3-CH_3)



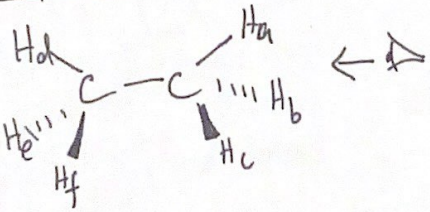


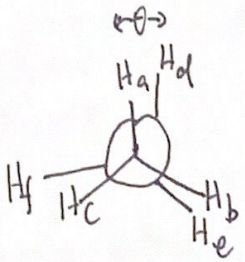
Ha and Hd are "anti" (opposite)

Staggered
$\theta = 60°$

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

Eclipsed Ethane





Eclipsed
$\theta = 0°$

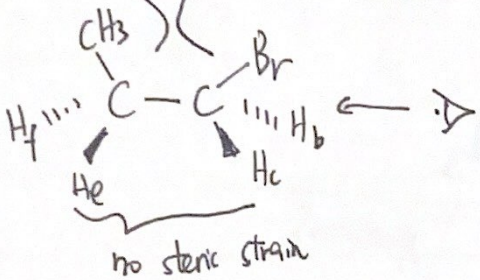
"H" atoms are small, so they never hit each other, even when eclipsed. → Ha and Hb above don't "clash" in space.

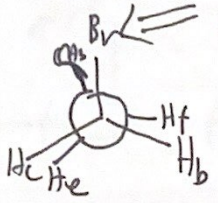
No steric strain between 2 H atoms!

art bigger atoms or groups (eg. Cl, Br, $-CH_3$, $-C_6H_5$)

Can "clash" or hit each other in space.

steric strain! ↳ "steric strain (Non-Bonded strain)

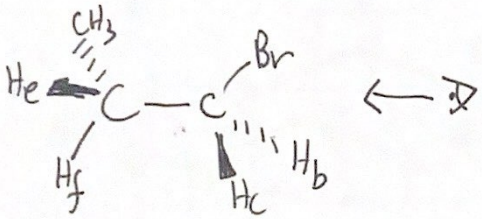


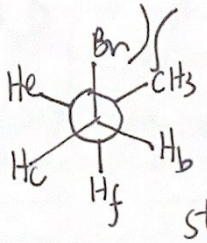


Eclipsed, $\theta = 0°$, torsional strain!

Do these two H atoms hit each other? No

Do -Br and $-CH_3$ hit each other? yes.





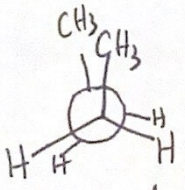
← steric clash

"Gauche"

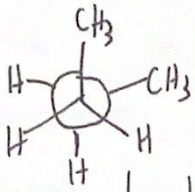
staggered, $\theta = 60°$

No torsional strain,

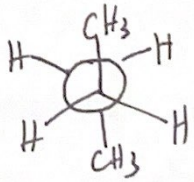
but steric strain still.



eclipsed butane



Gauche butane

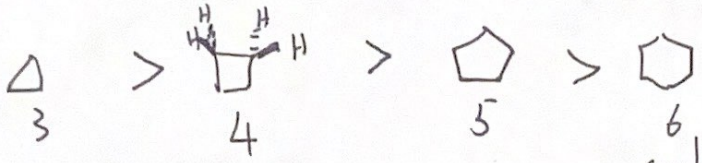


Anti-staggered butane

Torsional strain:	Yes!	No	No
steric strain:	Yes!	Yes!	No

Ring / Angle strain → in a ring

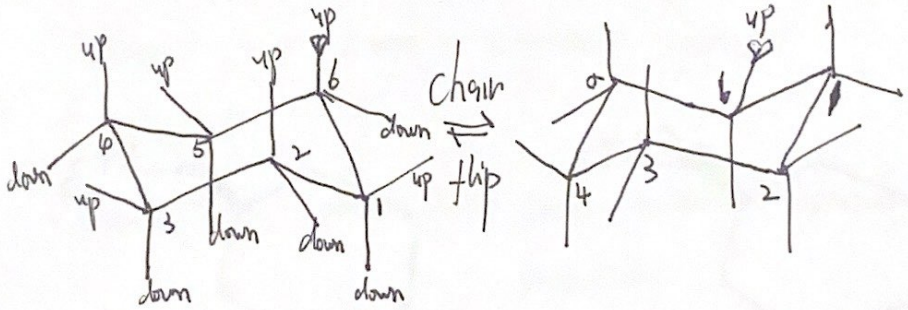
atoms in ring:



cyclohexane, no ring strain

Increasing ring strain

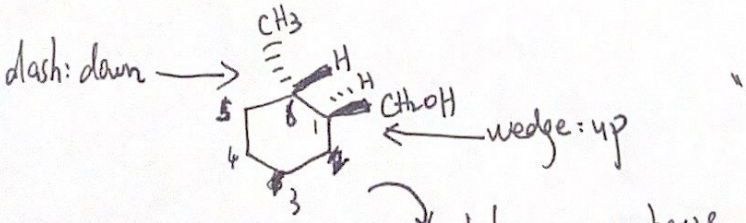
chair conformation



Large group prefer to be equitorial

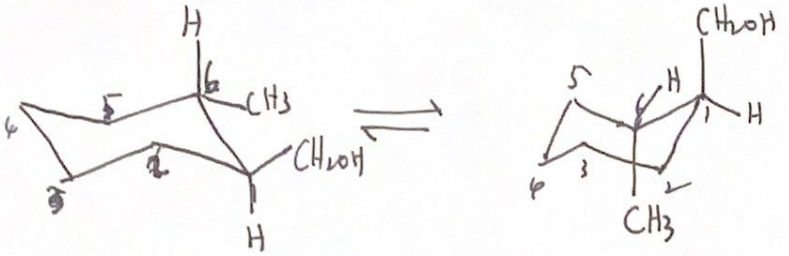
Chair flip is not a "pancake" flip.
will interconvert axial and equitorial groups

Eg: Draw 2 chair conformation for the following molecule and determine which one is favored



"trans"

clock-wise numbering



two groups are both equitorial

✓ more stable!

two groups are both axial

Stereochemistry

Isomer → same chemical formula

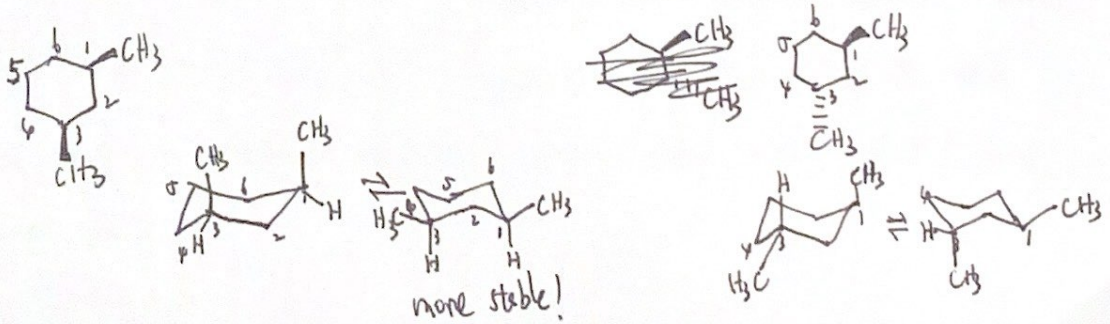
$C_4H_{10}O$

- Constitutional isomer → 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.

Ex:



more stable!