(9) **Today**

Chap 4 Cycloalkanes
Section 4.1 Naming Cycloalkanes and Halogen Substituents

Section 4.2 cis-trans isomerism Chap 4 Cycloalkanes

Sections 4.3 – 4.8 Stability of Cycloalkanes and Conformations of Cyclohexanes

Next Class (10)

Sections 5.1 – 5.5
Chirality and Determining the Configuration of Chiral Centers

Sections 5.6 – 5.12
Diastereomers, N,P, and S, and Prochirality

(11) **Second Class from Today**

Sections 5.1 – 5.5
Chirality and Determining the Configuration of Chiral Centers

Sections 5.6 – 5.12
Diastereomers, N,P, and S, and Prochirality

Third Class from Today (12)

Sections 5.11, 5.12
Prochirality

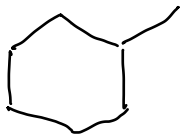
Chap 6

Rework Test 1 by Monday June 9.

There are no classes on Thursday, June 19th.

Cycloalkanes

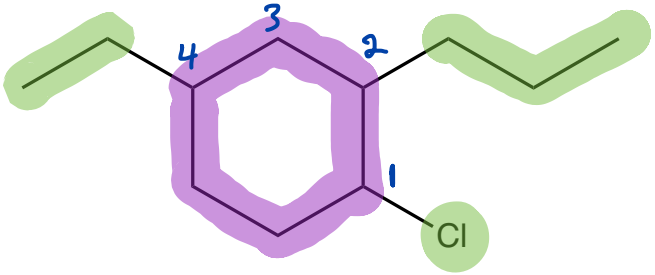
- Determine the name of the parent alkane
  - Ring is the parent hydrocarbon unless the alkyl substituent has more carbons; in that case the acyclic part becomes the parent hydrocarbon
  - cyclo(number of carbons)ane
    - cyclohexane a ring of 6 C atom
    - cyclopentane
- Cite the name of substituent before the name of the parent cycloalkane
  - one substituent, no need to give it a number
  - two substituents
    - alphabetical order
    - first substituent is given the number 1
    - numbers counted (clockwise or counterclockwise) to give lowest 2nd substituent number
  - more than two substituents
    - not necessarily in alphabetical order
    - starting point (substituent with number 1) and direction of the counting (clockwise or counterclockwise) is decided by finding the combination that gives the lowest possible numbers for all of the substituents

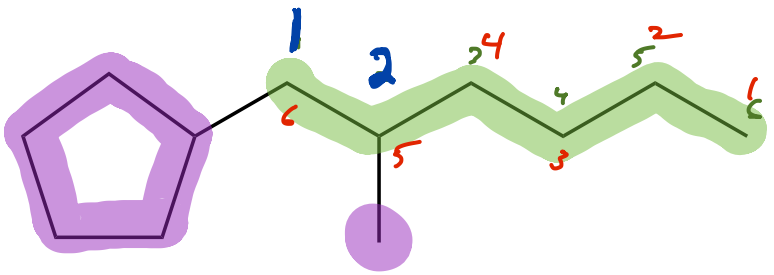


methylcyclohexane

Practice Nomenclature

Section 4.1





longest chain/ring:

2 or 3

6 in ring

parent alkane name

hexane

functional group (?) and position:

cyclohexane

substituent names

2 carbon long group → ethyl

3 carbon long group → propyl

a chlorine atom → chloro

substituent positions

1, 2, 4 or ~~1, 4, 6~~

full name:

1-chloro-4-ethyl-2-propylcyclohexane

longest chain/ring:

6 5

parent alkane name

hexane

functional group (?) and position:

not cyclohexane

substituent names

1 carbon long group → methyl

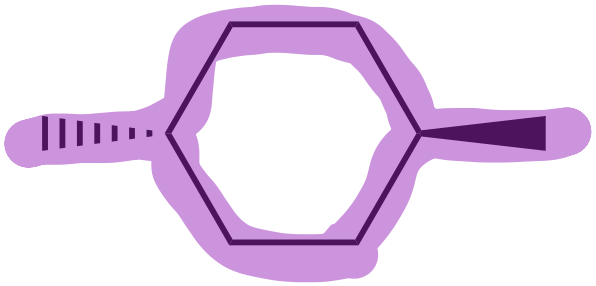
5 carbon ring group → cyclopentyl

substituent positions

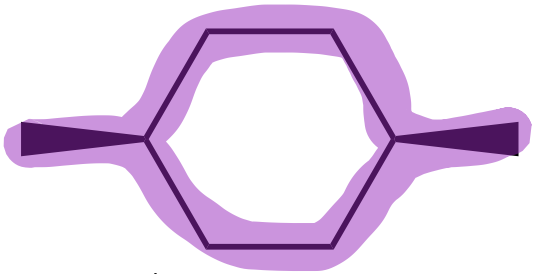
1, 2 ~~5, 6~~

full name:

1-cyclopentyl-2-methylhexane



trans - dimethylcyclohexane



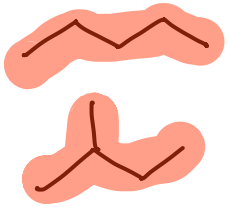
cis - dimethylcyclohexane

cannot be interconverted by rotation

isomers
same formula
⊞

constitutional/
structural
isomers

same formula
different
connectivity



stereoisomers
same formula, same connectivity,
different 3D relationship

conformational
isomers

rotation about
single bonds

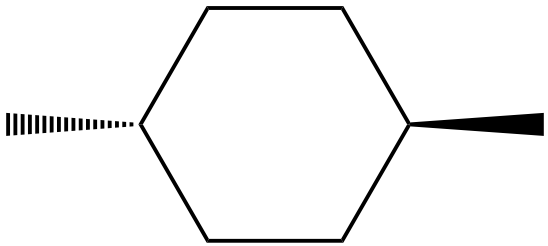
amine inversion

⊞

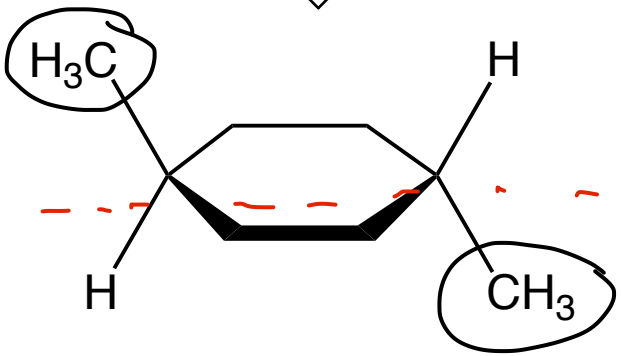
configurational
isomers

cis/trans
isomerism

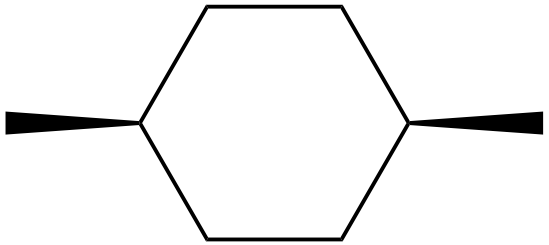
chirality centers



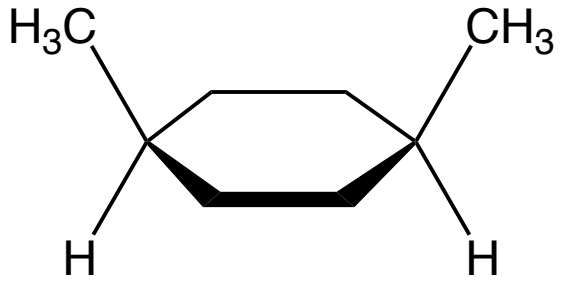
rotate ⇓ 90°



methyl groups are on opposite sides of the plane of the ring trans



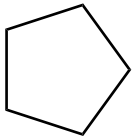
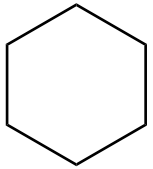
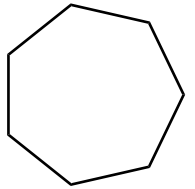
rotate ⇓ 90°



methyl groups are on same side of the plane of the ring cis

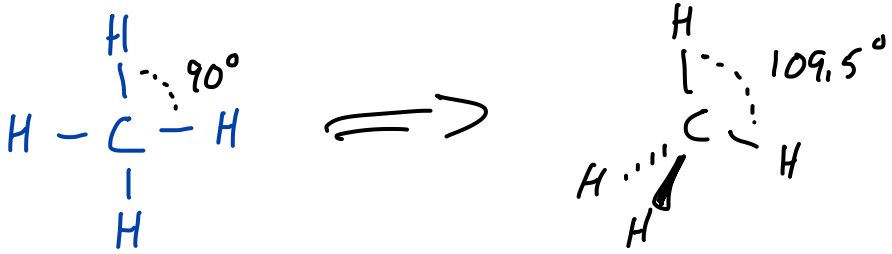
cannot be interconverted by rotation
can be separated from each other



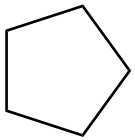
60 90 108 120 128

incorrect hypothesis these don't have to be planar

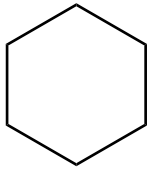


60

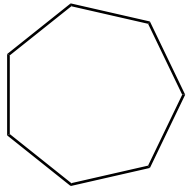
~~90~~



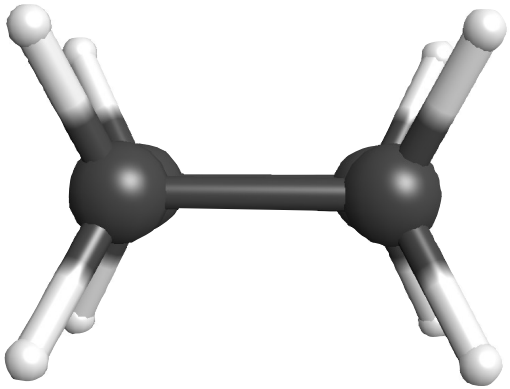
~~108~~



~~120~~

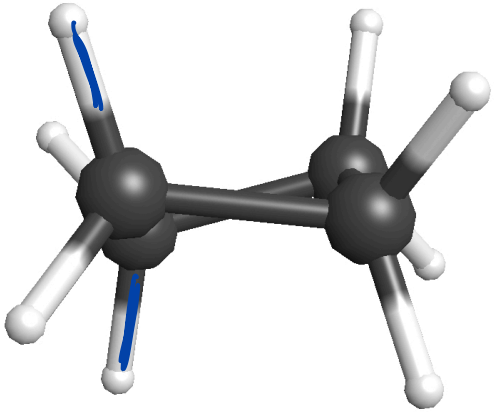


~~128~~

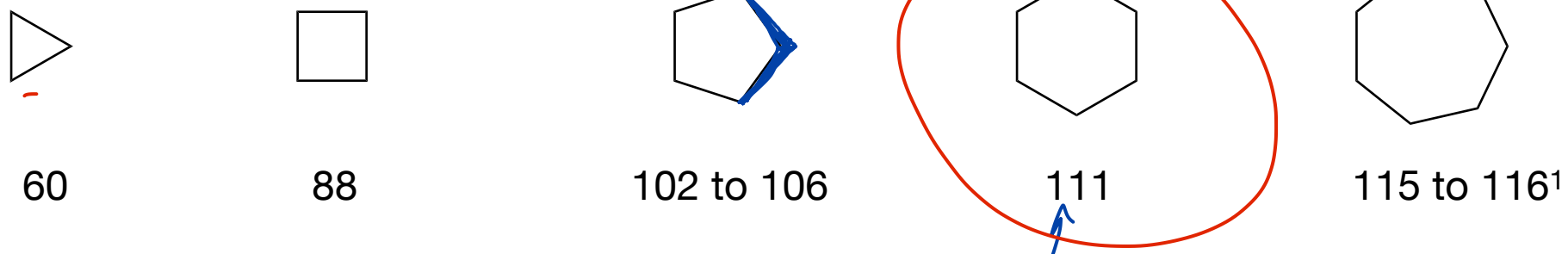


eclipsing geometry

2 atoms are not in the same plane



now the geometry is slightly staggered



60 88 102 to 106 111 115 to 116[1]

most stable cycloalkane

e⁻'s in these orbitals cannot get directly between the two C atoms.... not as low in E... they are higher in E.... more reactive

react more like alkenes than alkanes

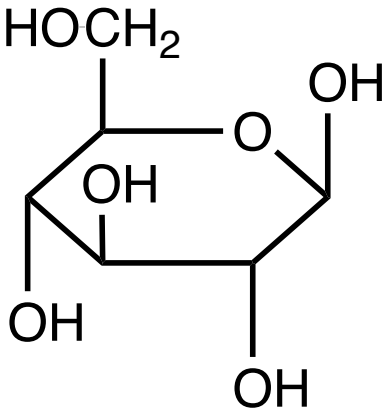
e⁻'s between two ⊕ charged nuclei... low in E

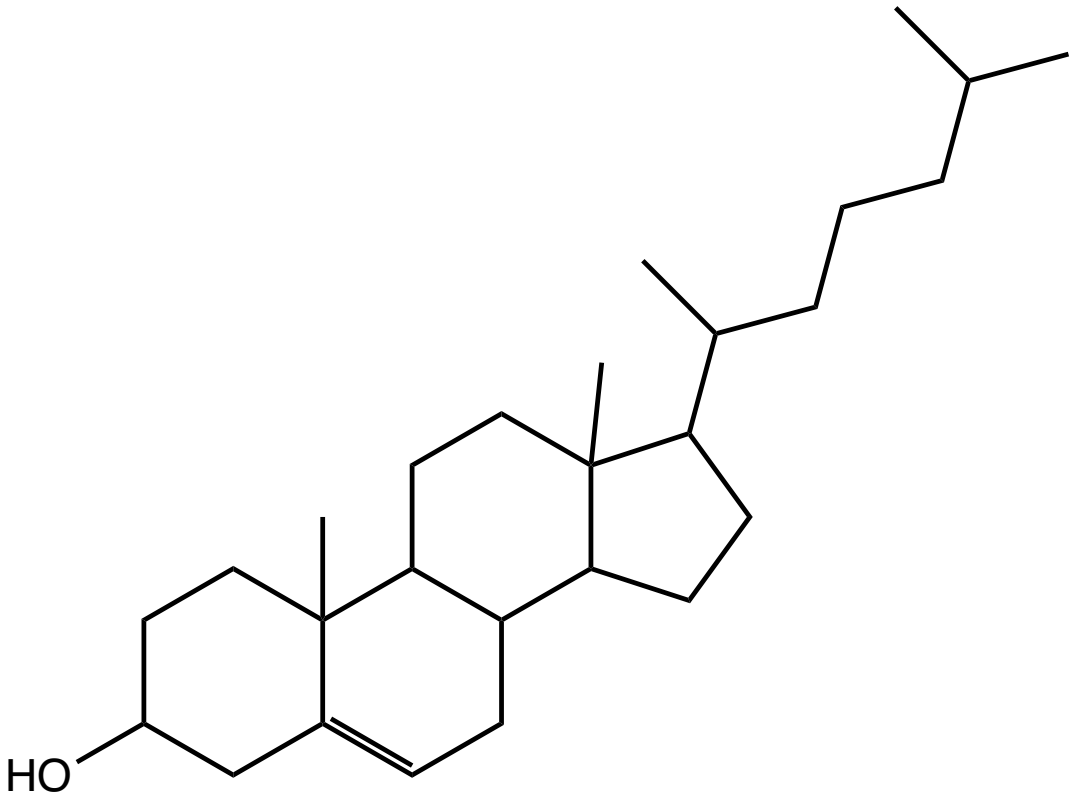
sp^3 sp^3

[1] Based on quick mechanics calculations in WebMO

Why?

six-membered rings appear a lot in nature





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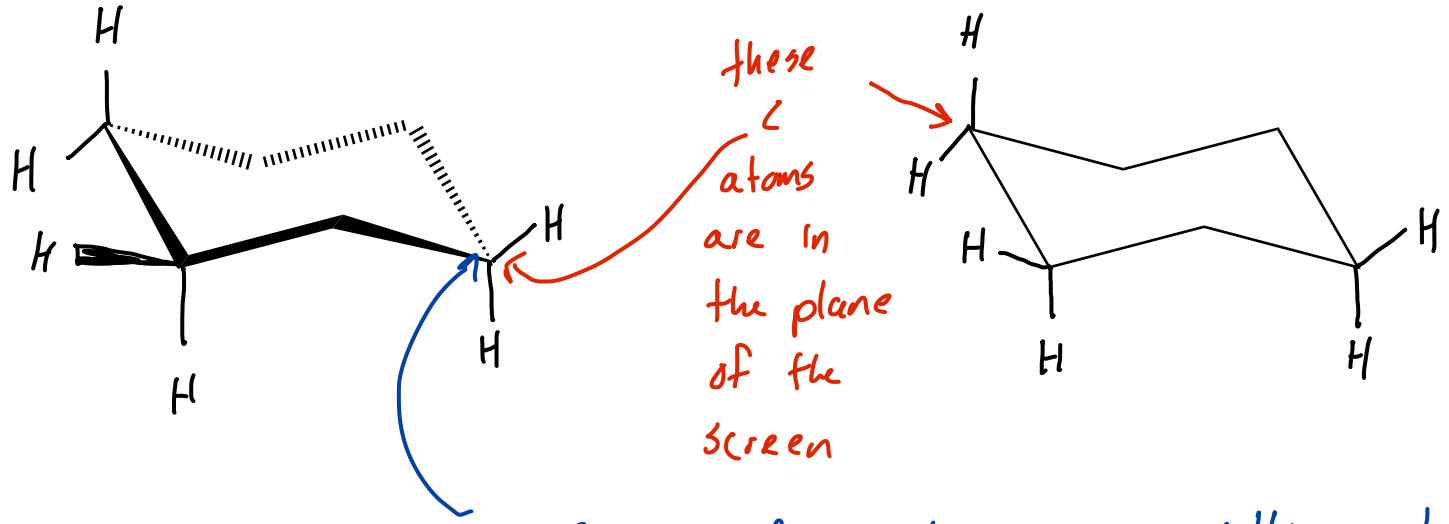
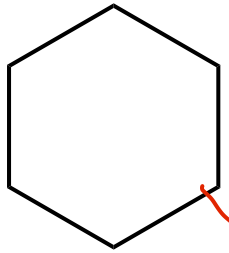
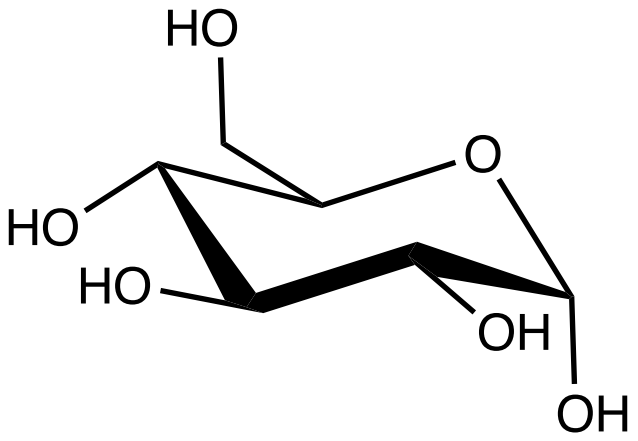


111° bond angles ... very little angle strain
all geometries are staggered ... no torsional strain



120° bond angles ... angle strain
all geometries are eclipsed ... lots of torsional strain



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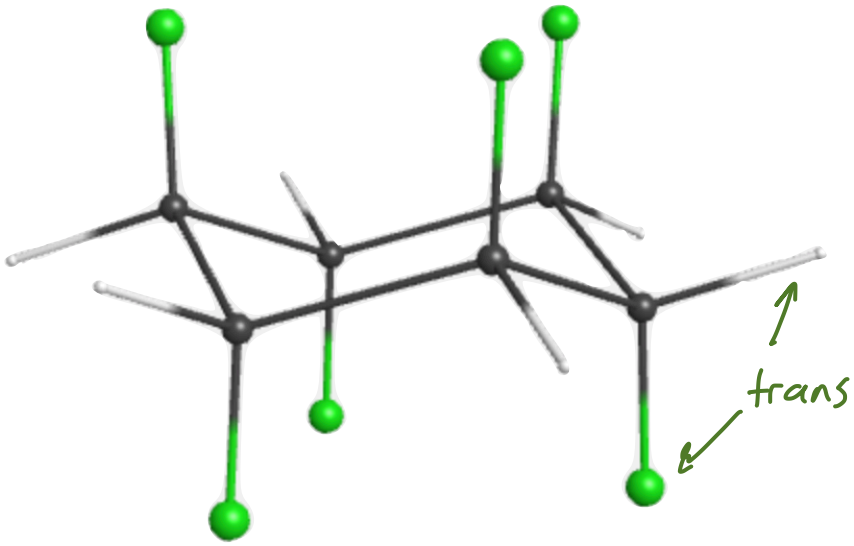
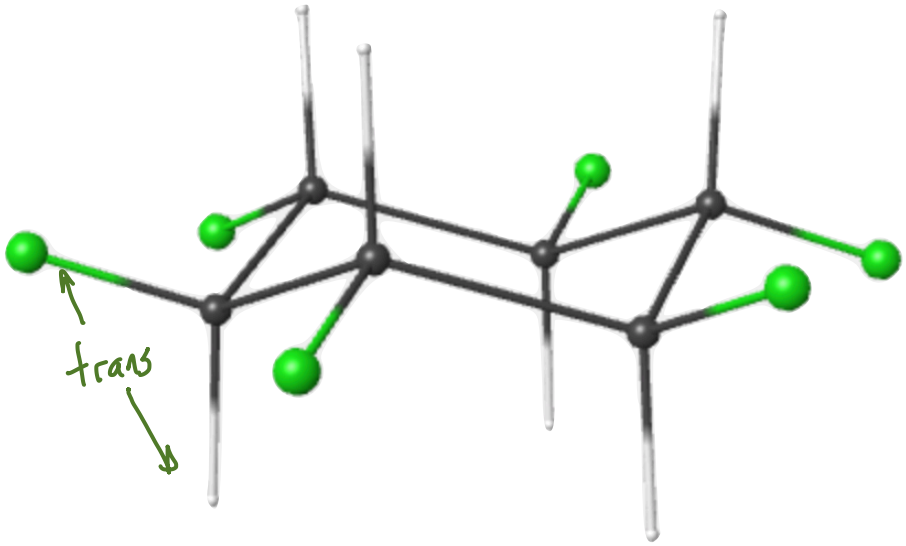
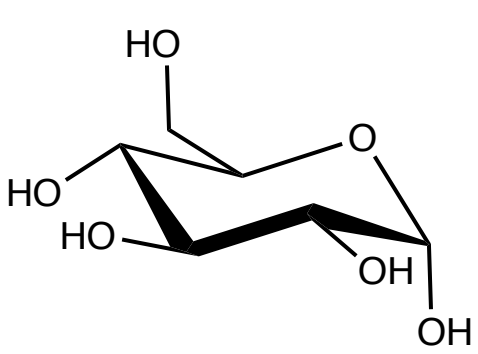
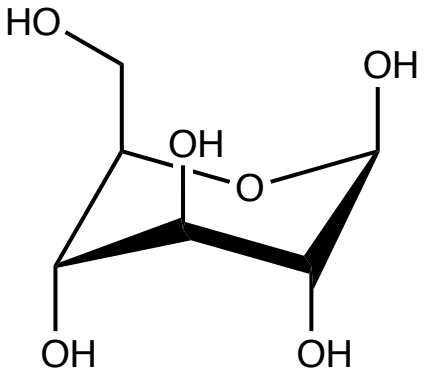

trans

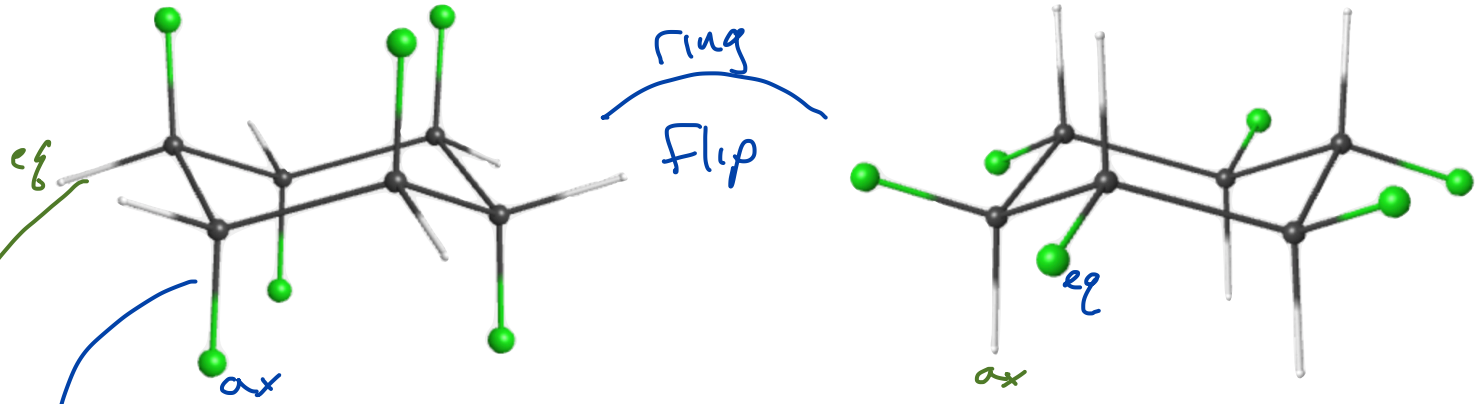

trans

Why?



ring flip





straight up and down ones are axial

ring flip → becomes equitorial

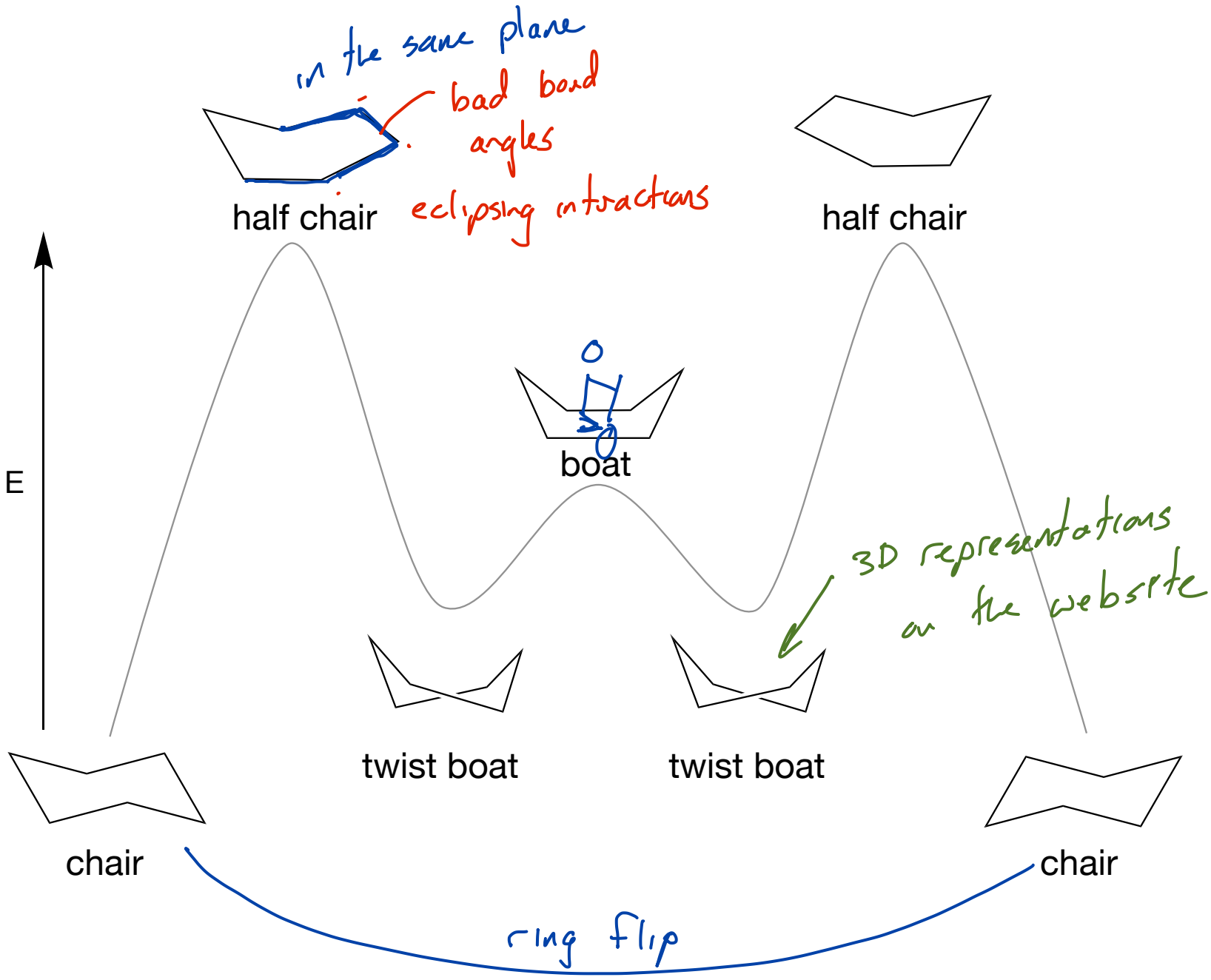
pointing out the sides equitorial

ring flip → became axial

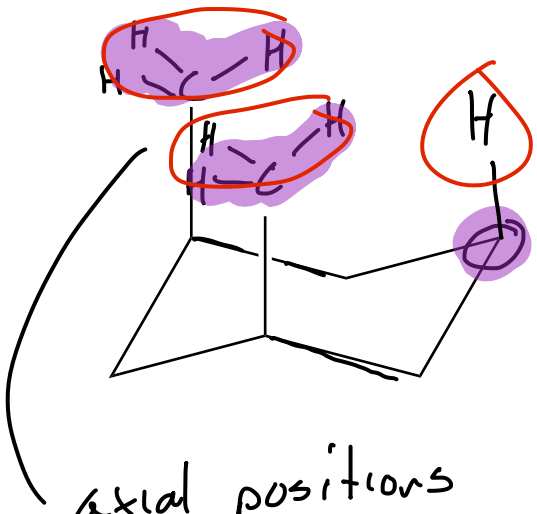
★ cis + trans relationships do not change when a ring flip happens. ★

cis substituents remain cis to each other

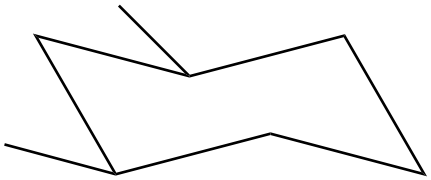
trans substituents remain trans to each other


in the same plane
bad bond angles
eclipsing interactions
half chair
half chair
boat
E
3D representations on the website
twist boat
twist boat
chair
chair
ring flip

substituents are lower in E when in the equitorial positions



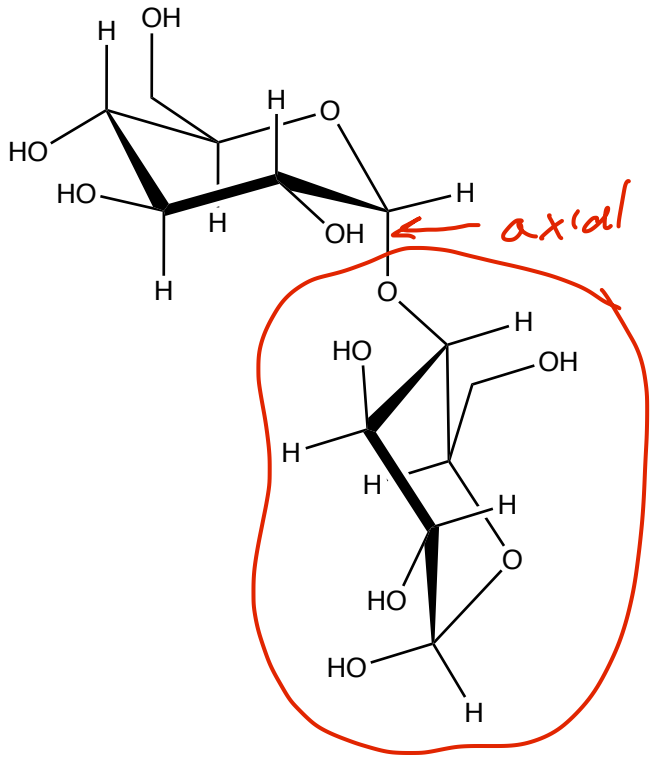
ring flip



axial positions experience gauche interations with ring steric interactions (repulsion) between axial positions

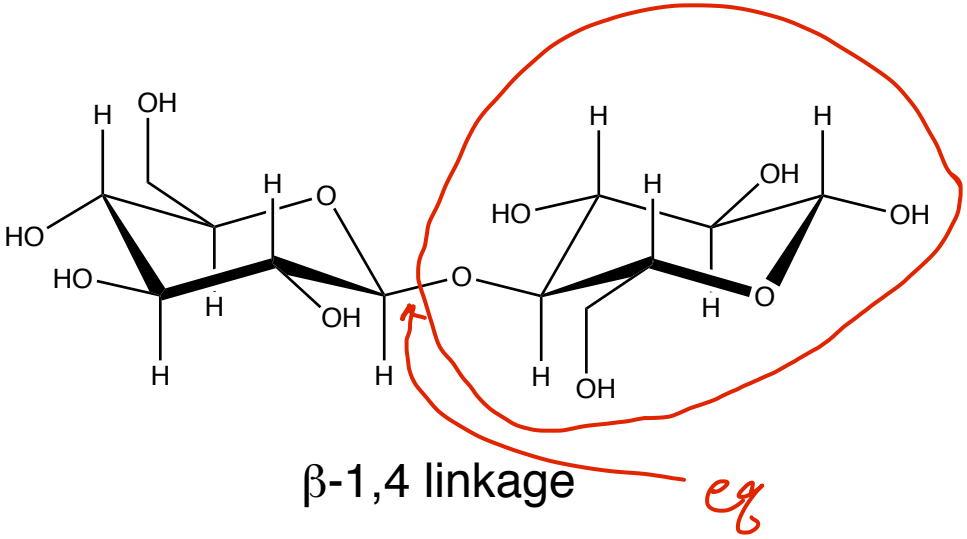
lower energy structure equitorial positions put substituents farther away from the other atoms on the ring

https://www.westfield.ma.edu/cmasi/organic/cyclohexanes/sub_cyclohexanes-plain.html



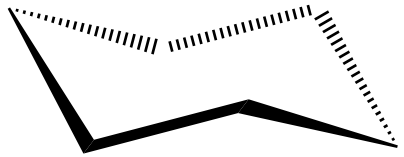
α-1,4 linkage

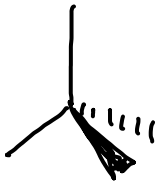
starch & glycogen



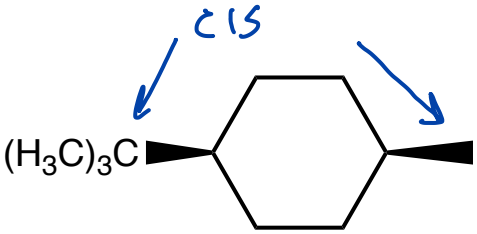
β-1,4 linkage

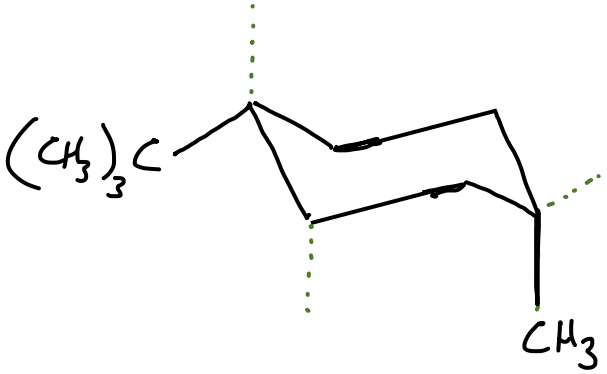
cellulose

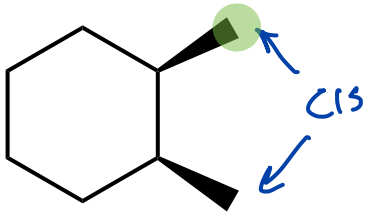


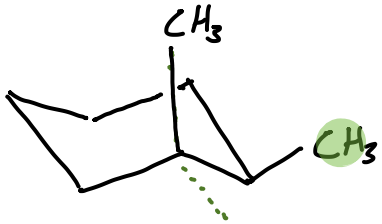


Things to keep in mind while drawing cyclohexane conformations

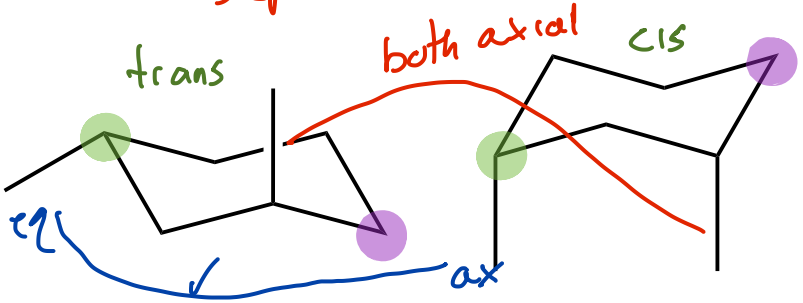




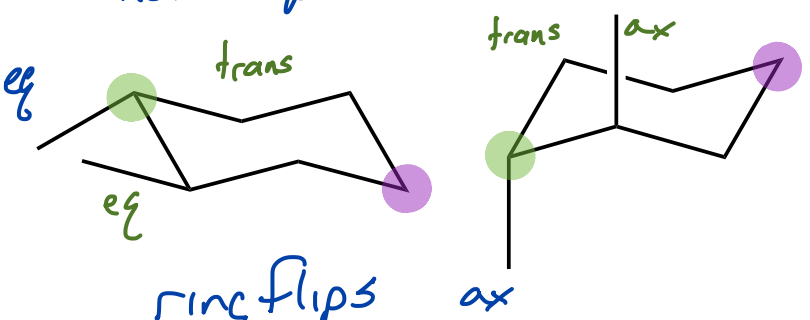




separable stereoisomers

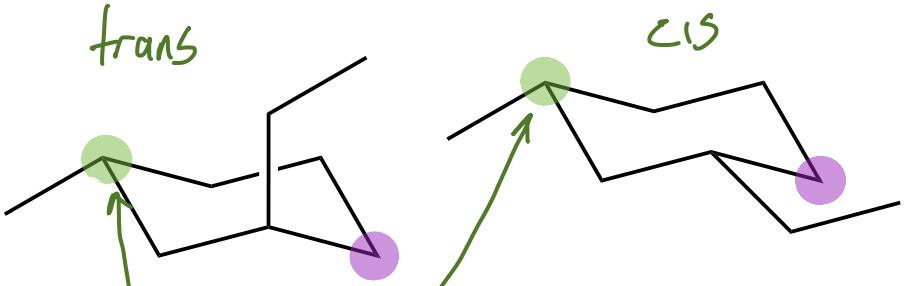


not separable



ring flips

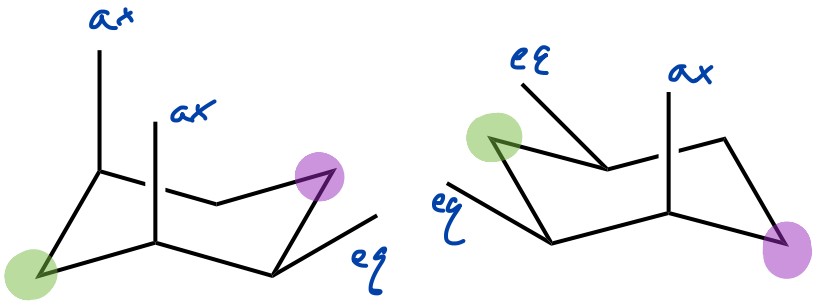
substituents in same positions on ring
all axial position became equatorial + vice versa } if yes .. ring flip



green position didn't change

eq + ax didn't switch

separable stereoisomers



ring Flip

not separable