5.12

V. Alkanes

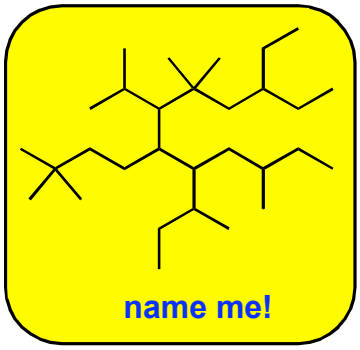
G. Cycloalkanes

1. Nomenclature
2. Stereochemistry
3. Ring Size and Strain

H. Cyclohexane

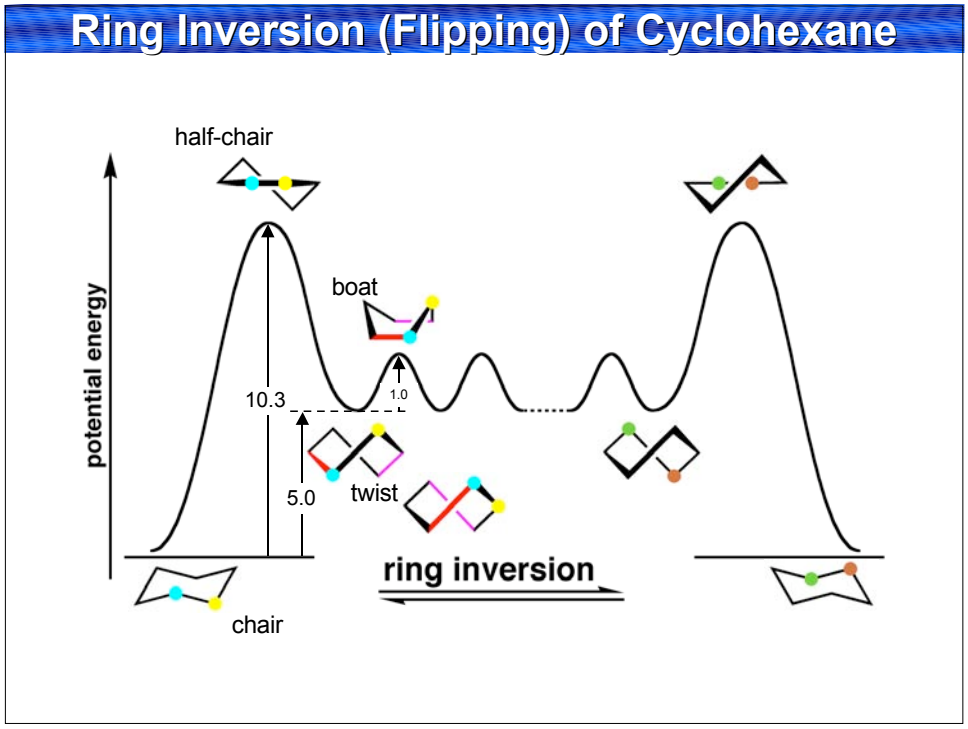
1. The Chair
2. Ring Flip
3. Monosubstituted
4. Disubstituted

I. Polycyclic



Naming Cycloalkanes

1. Find parent (ring or chain, depending on which is larger).
2. Label point of attachment of alkyl, halo, etc. as C1.
3. Continue numbering so that the second substitutent is the lowest possible number.
4. If 2 or more groups could potentially get the same number, use alphabetical order as a tie-breaker.



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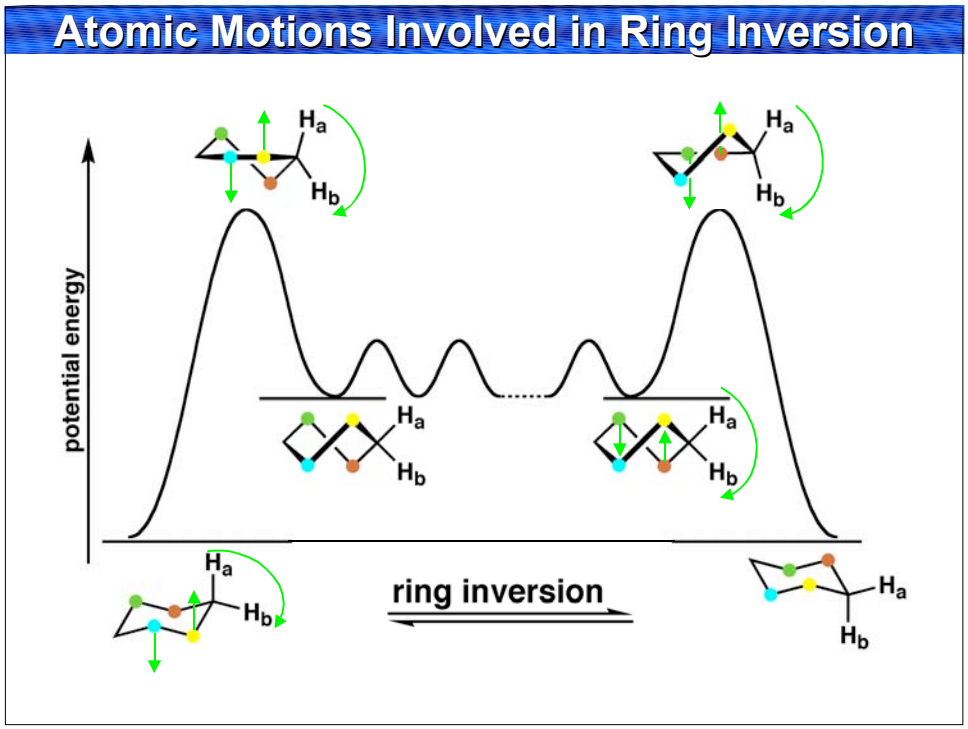

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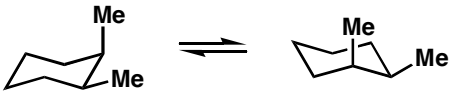
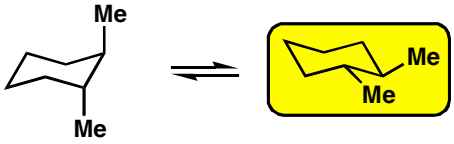
Disubstituted Cyclohexane

If 2 substituents are on cyclohexane the lowest energy conformation:

a) Has both substituents equatorial (if possible)
b) The group with the largest A value equatorial
c) *t*-Bu is NEVER axial!

1,2-*cis* 

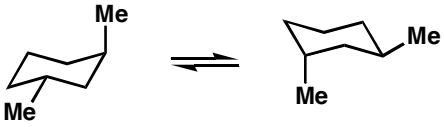
1 ax. 1 eq. versus 1 ax. 1 eq.
same energy

1,2-*trans* 

2 ax. versus 2 eq.
all equatorial preferred

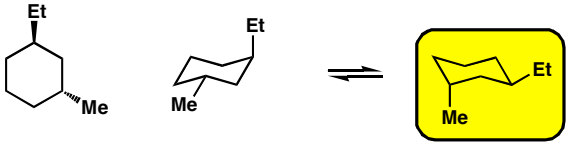
1,3-*cis* 

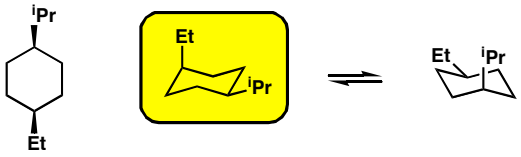
2 ax. versus 2 eq.
all equatorial preferred

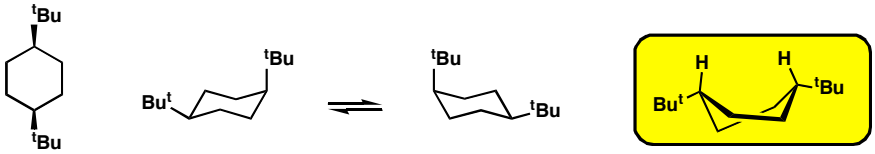
1,3-*trans* 

1 ax. 1 eq. versus 1 ax. 1 eq.
same energy

Disubstituted Examples

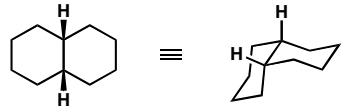




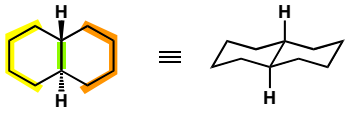


Polycyclic

1. Fused rings



cis-decalin — can ring flip



trans-decalin — can't ring flip (locked!)

bicyclo[4.4.0]decane

2. Bridged rings

conformationally locked

bicyclo[2.2.1]heptane

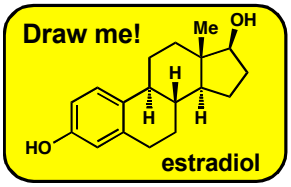
3. Spirocyclic rings (rare)

spiro[4.4]nonane

Nomenclature:

a. Prefix = bicyclo or spiro
b. [Number] = number of carbons between bridgeheads, descending order
c. Suffix = total carbons -ane

Draw me!



estradiol

Drawing Cyclohexane Chairs

Steps 1–3: Draw three pairs of parallel lines as shown

(1) (2) (3)

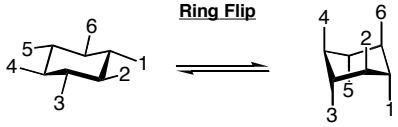
Steps 4–6: Draw equatorial bonds parallel to ring bonds in bold

(4) (5) (6)

Steps 7,8: Draw axial bonds as vertical lines below and above ring.

(7) (8)

Ring Flip



- **Interconverts equatorial and axial substituents.**
- **Energetic barrier = 10 kcal/mol; occurs rapidly at room temperature.**

Substituted Cyclohexane

equatorial: C–X bond **anti** to ring bonds

axial: C–X bond **gauche** to two ring bonds

- This means that axial groups experience **1,3-diaxial interactions**; "bump into" other axial groups.

- **EQUATORIAL PREFERRED**

A-Values to Remember

–X	A-Value
$-CH_3$	1.74
$-CH_2CH_3$	1.8
$-CH(CH_3)_2$	2.1
$-C(CH_3)_3$	5.4
–CN	0.2
–OH	1.0
–Cl	0.5
–Br	0.6

- **A-Value** = magnitude of equatorial preference