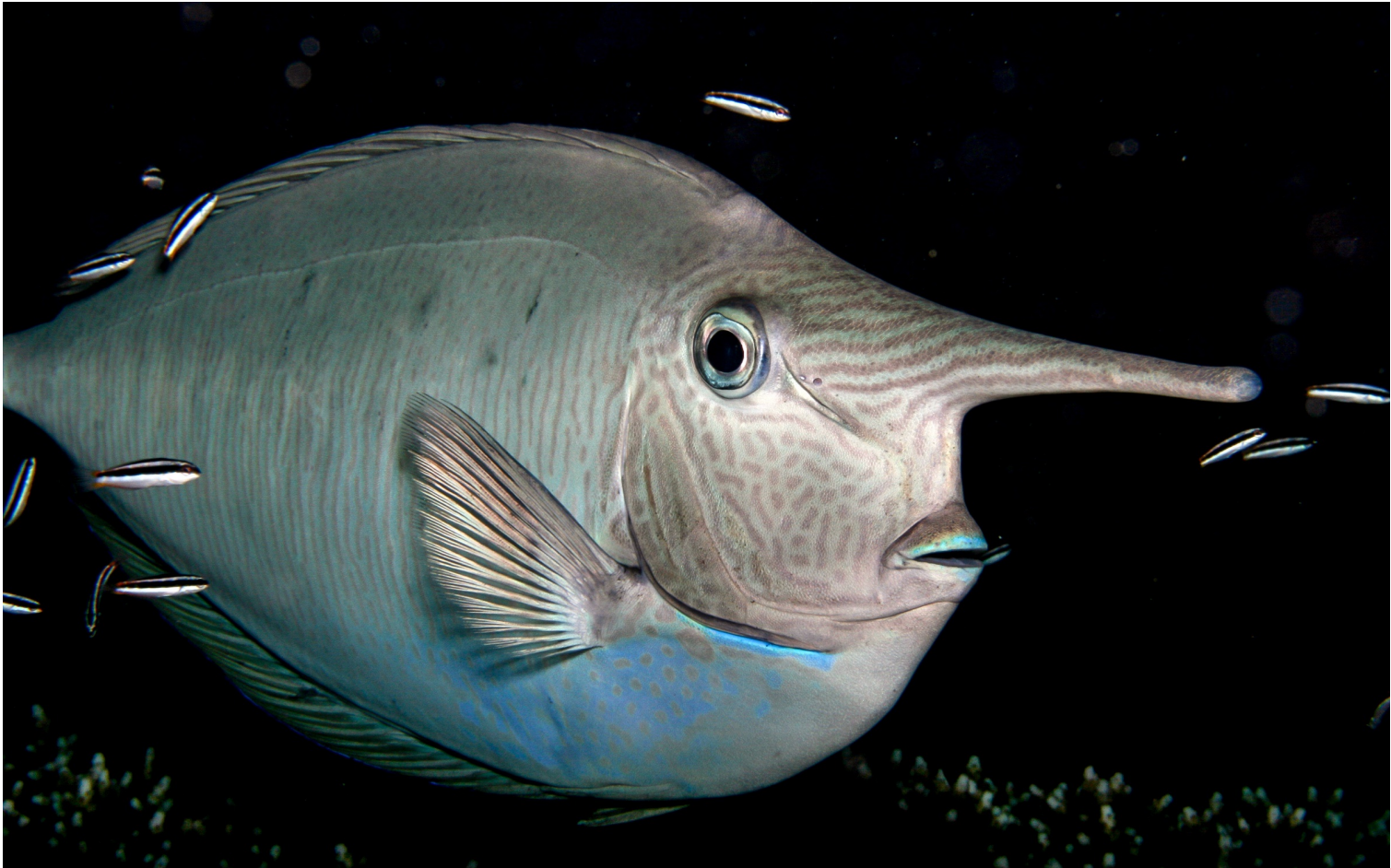




What you need to know

Important concept $\rightarrow$ Energy and stability are relative terms that are related to each other $\rightarrow$ "relative" because they need comparisons to make sense

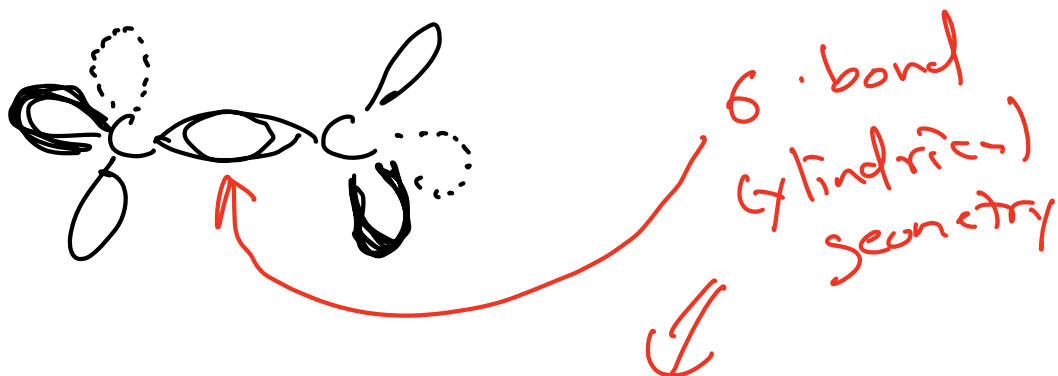
A molecule with higher energy is less stable

A molecule with lower energy is more stable

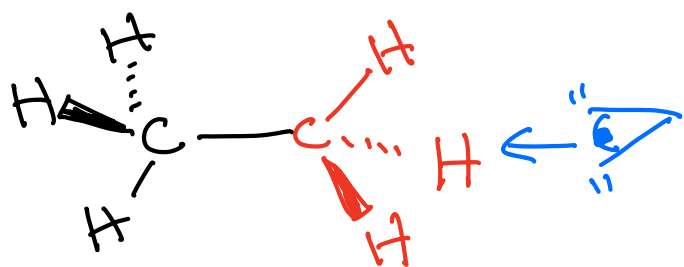
Strain $\rightarrow$ increases molecular energy and decreases stability

$\Rightarrow$ Molecules are found predominantly in their lowest energy (most stable) form.

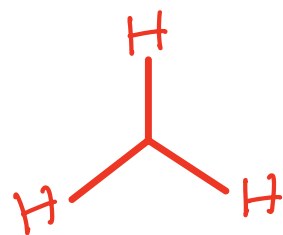
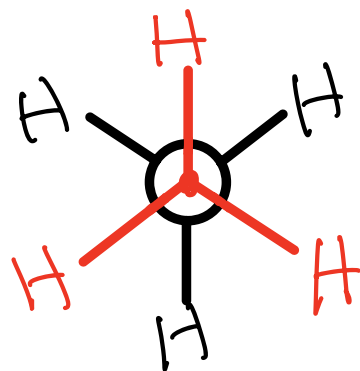
Carbon-Carbon sigma bonds rotate rapidly at room temperature



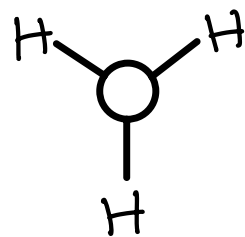
It does, not get weaker as it rotates.



Newman Projection

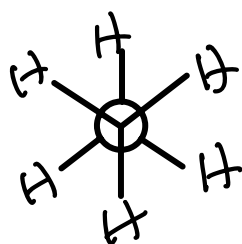


Carbon in 'front'

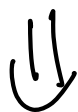


Carbon in back

Two extremes

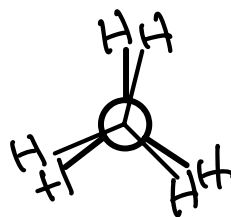


Staggered
Conformation



More stable

minimal torsional strain



Eclipsed
Conformation



Less stable

maximum
torsional strain

Torsional Strain $\rightarrow$ a complex effect
based on

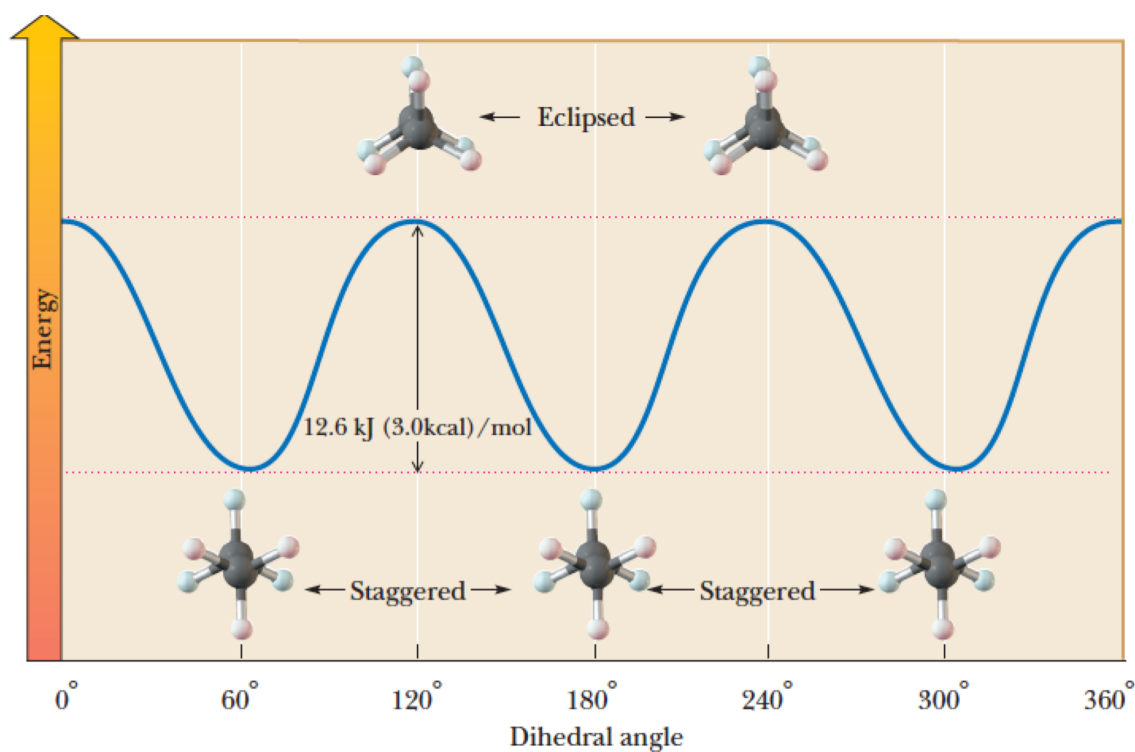
TIME
CAPSULE



we discuss
in chapter 6

hyperconjugation
that introduces strain
unless the H atoms
are in the staggered
geometry

The ethane molecule rotates freely at room temperature, but because of torsional strain it spends most of its time in the staggered conformation

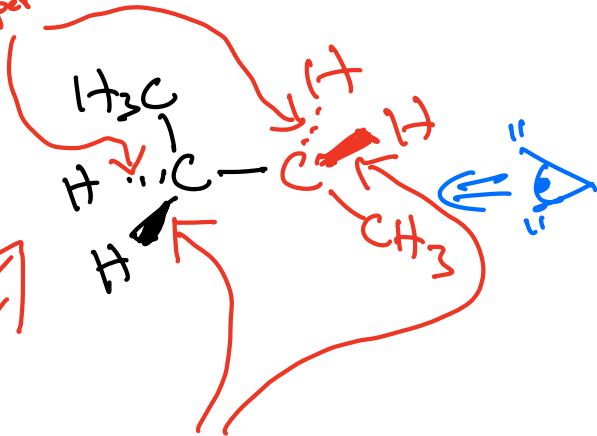


New type of strain $\rightarrow$ important for
alkanes of 4 or more
carbon atoms

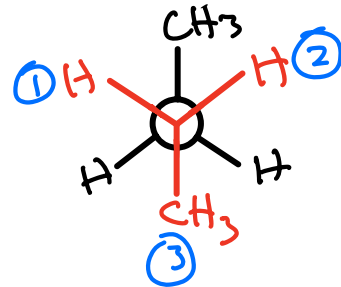
Steric strain $\rightarrow$ strain caused when
atoms "crunch"
into each other

Butane $\rightarrow$ 4 carbon atoms
3 different staggered
conformations

These atoms are
positioned away
from us - behind
the plane of the
paper

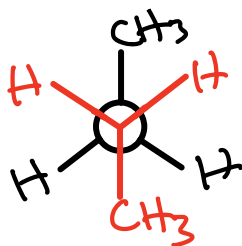


These atoms are
positioned toward
us - in front of the
plane of the paper



Bonds drawn with
normal lines indicate
the atoms positioned
in the plane of the
paper.

3 different staggered conformations

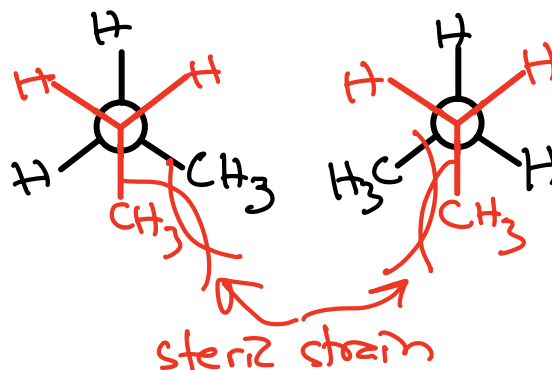


Anti

(methyl) groups are
as far apart as
possible

No steric strain

Lower energy



Gauche

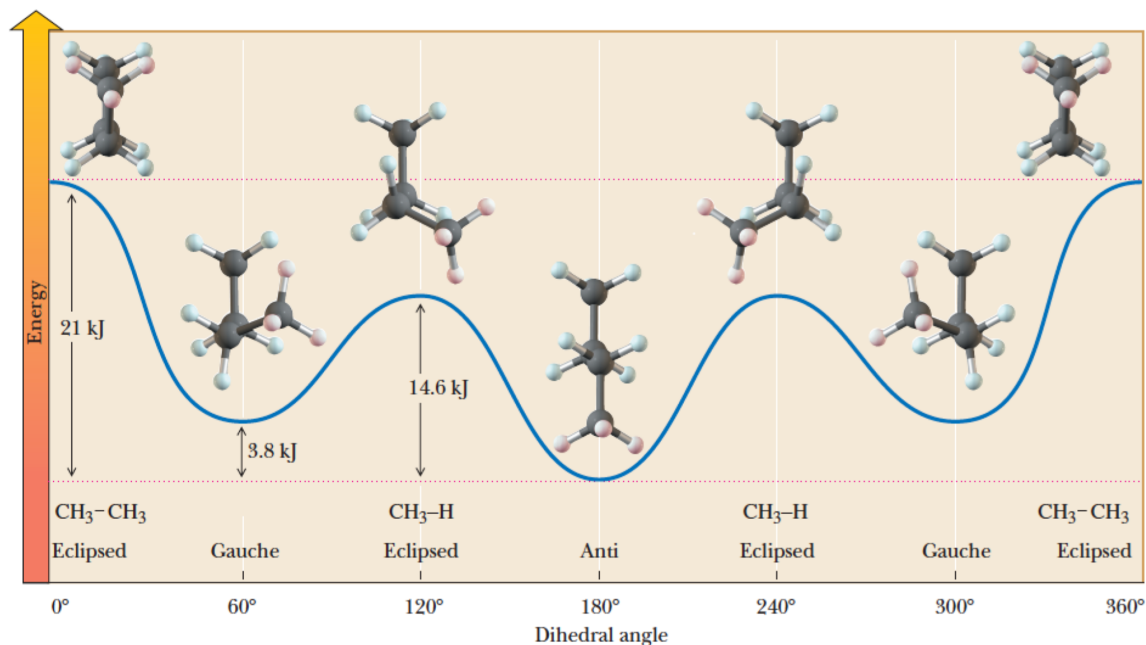
(methyl) groups
are adjacent

Steric strain

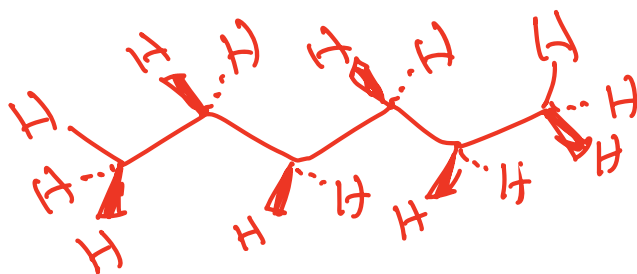
because "poor"

methyl groups
crunch into each
other

Higher Energy



Important consequence → for longer alkanes → *alkane chains exist primarily in a "zig zag" conformation so that all the bonds are staggered anti most of the time*



Dynamizes $\rightarrow$ heat in molecules causes the amplitude of bond vibrations to increase

Very disorganized bond rotation

Vibrations and rotations are coupled in molecules $\rightarrow$ vibrations that lead to bond rotations

Angle strain $\rightarrow$ present any time an angle around an sp^3 C is different than 109.5°

$\rightarrow$ Happens in ring structures

Cycloalkanes

Cyclopropane

↓
Highly strained



High angle strain
and
high torsional strain

Cyclobutane

↓
Highly strained

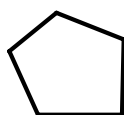


Not flat

Angle strain
Torsional strain
"puckers" to relieve
some strain

Cyclopentane

"Pucker" to create
an "envelope"
conformation



Very little
strain

Little angle
strain but
some torsional
strain

Cyclohexane $\rightarrow$ most stable cyclohexane

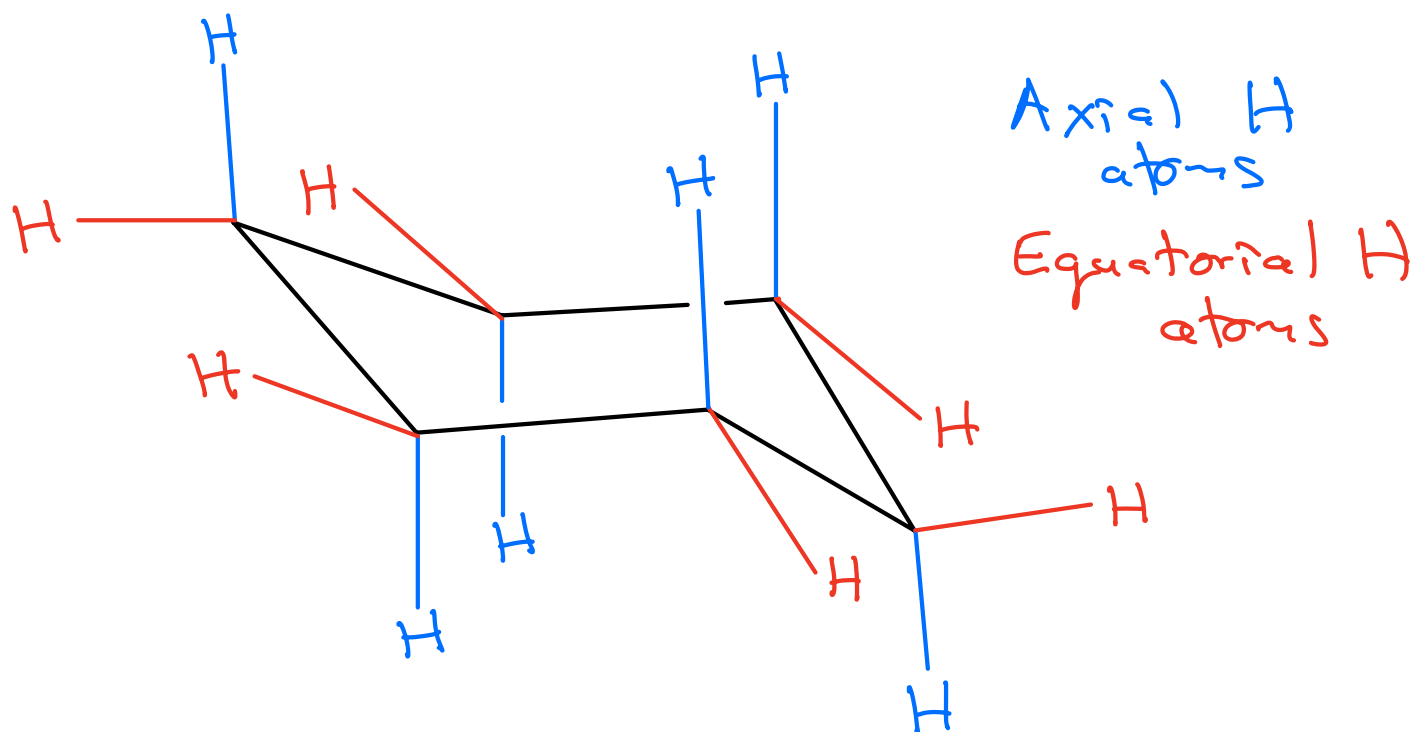
$\hookrightarrow$ Adopts a chair conformation

$\Downarrow$
Minimal angle strain

$\Downarrow$
No torsional strain

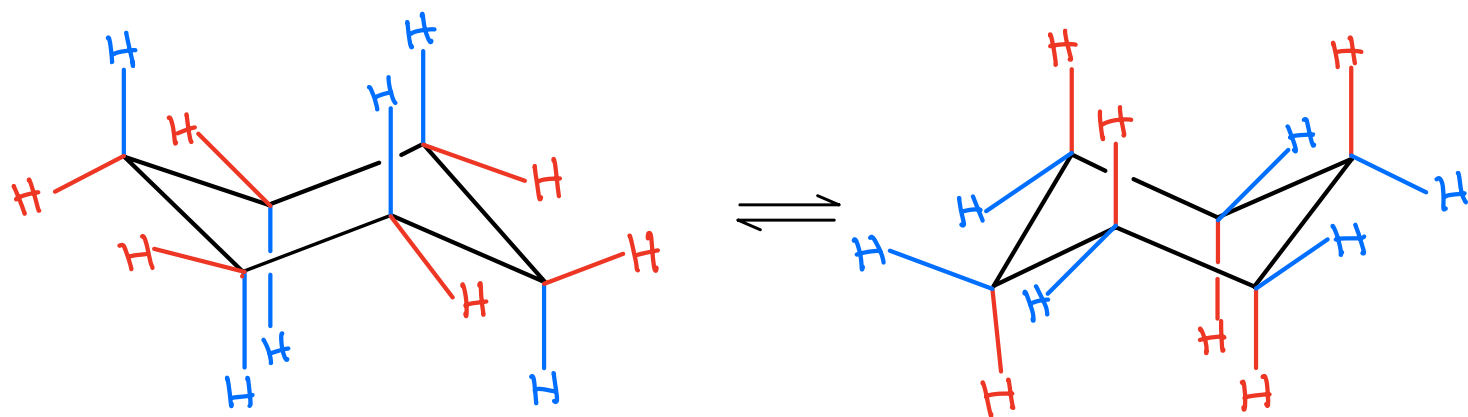
You will need to know how to draw a **great** chair cyclohexane

$\Rightarrow$ "Keep It Parallel"



There are two kinds of H atoms in a chair cyclohexane - axial (blue) and equatorial (red) $\rightarrow$ these are different chemical environments

The cyclohexane chair can "flip"
at room temperature



When the chair flips - the axial H
atoms become equatorial and the
equatorial H atoms become axial.
As chairs flip, they go through a
boat-like conformation

In a cyclohexane chair conformation, any group larger than an H atom will prefer to be equatorial to avoid steric strain ("crunching") → the larger the group R, the greater the preference for being equatorial.

