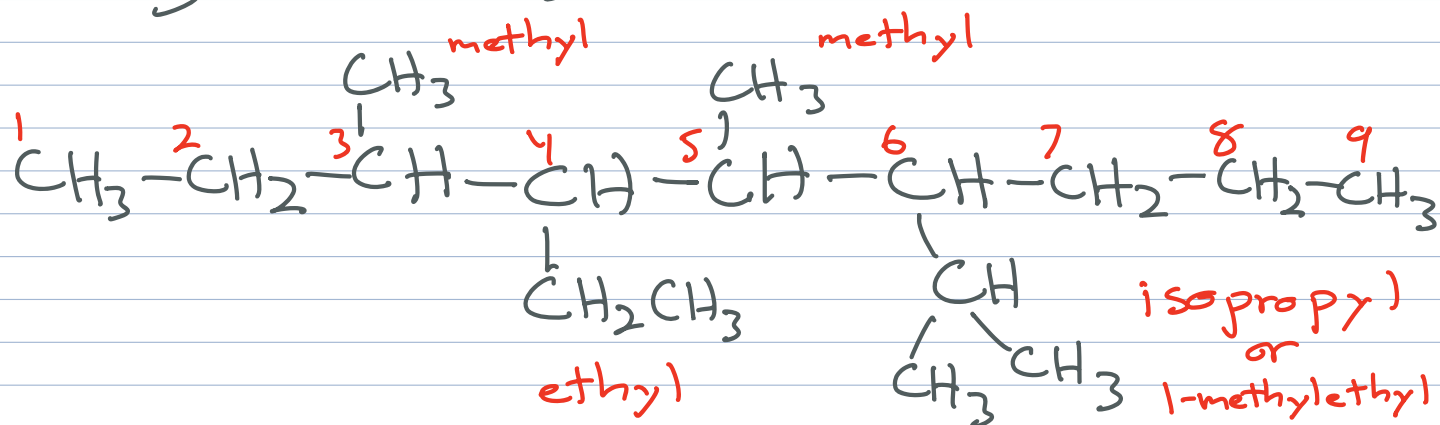




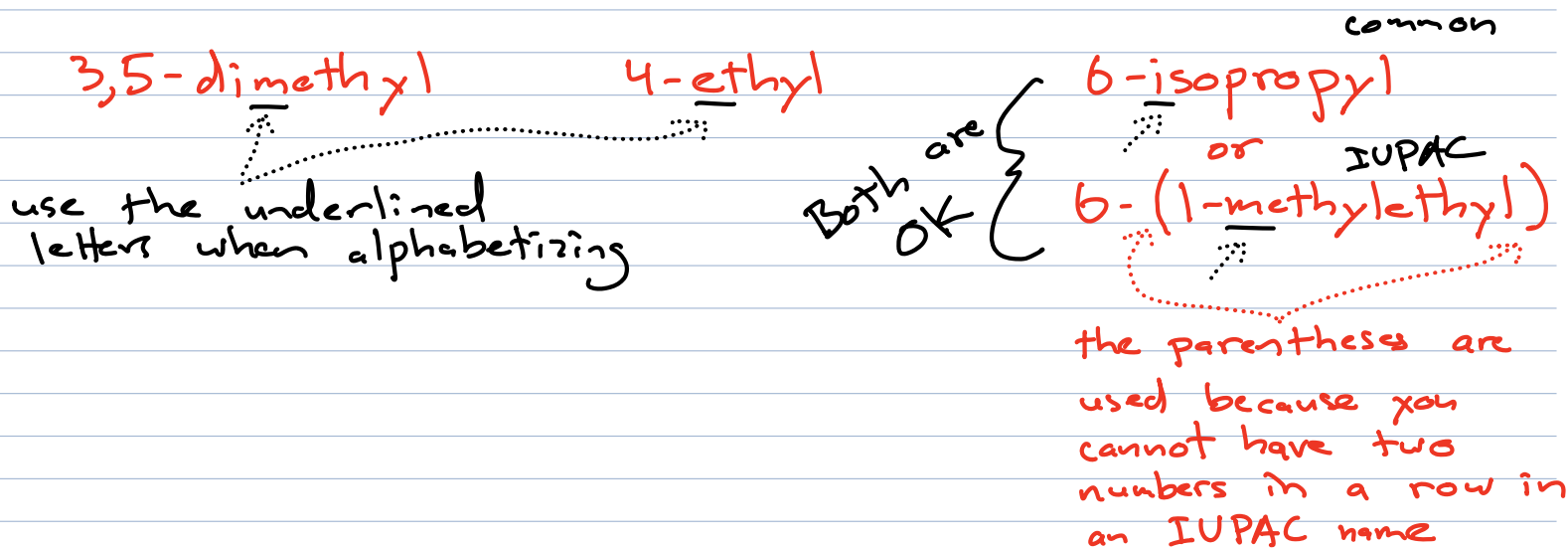


Putting it all together:



nonane \rightarrow 9 carbons in parent chain

number from left to right so the first group encountered has the lower number (3 not 4)



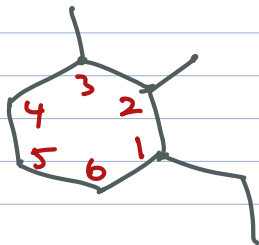
4-ethyl-6-isopropyl-3,5-dimethylnonane

or

4-ethyl-3,5-dimethyl-6-(1-methylethyl)nonane

Both of these names are acceptable

Cyclic Structures



1-ethyl-2,3-dimethylcyclohexane

When there are more atoms in the ring compared to any of the substituents \rightarrow the

parent chain is the ring \rightarrow add "cyclo" to the parent chain name

Number the ring to give the lowest overall numbers (1,2,3 not 4,5,6).

If there is a tie the first substituent by alphabet gets the lower number

IUPAC PROCEDURE FOR NAMING ALKANES

Before you begin you must:

- 1) Memorize alkane chain names (Table 2.1)
 - 2) Memorize substituent names (Tables 2.2 and 2.3)
- [I apologize on behalf of all chemists for the crazy names you have to memorize. I wish I knew an easier way, but I do not!]*

START HERE

Locate Longest Continuous Carbon Chain and Count Number of Carbon Atoms. Find the Alkane Name that Corresponds to the Chain (ex. heptane, dodecane, etc.) and Write this Down Leaving Room in Front of the Name for More Writing. If There are Alkane Branches Continue, if Not You are Done. Go Have a Party.

Number the Main Chain Such that the First Substituent Will Be Branching Off from the Lowest Numbered Carbon (this is not as hard as it sounds since there are only two choices on which way to number, choose the origin as being closest to the first branch point). If There are Substituents in Equivalent Positions from Either End, the Lower Number Goes to the One that Comes First in Alphabetical Order.

Does Branch have Branching?

No Branching On Branch Itself

- 1) Count the Number of Carbon Atoms in The Chain
- 2) Find the Name Corresponding to that Chain Length
- 3) Change the Suffix from ane to yl. This is Name of the Branch.

Yes, Branch Has Branches Of Its Own

1) Does Entire Branch Group Have a Trivial Name? (isopropyl, isobutyl, neopentyl etc.)

Yes

No

Write Number of Main Chain Carbon at Branch Point then a Dash (-) Followed by Name of Branch All Preceding Original Main Chain Name as One Word

Use Same Rules as for the Rest of Alkane: Pick Longest Continuous Chain, Name Branches Including Numbers But Use Parentheses Around Branch Name
Ex. 6-(2,3-dimethylbutyl)dodecane

!!! =>

ADDITIONAL RULES

- 1) If a Molecule Contains Two of the Same Branching Alkyl Groups Use the Prefix di, if Three Use tri, if Four Use tetra, if Five Use penta, if Six Use hexa etc.

Ex. 2,3,4-trimethylhexane

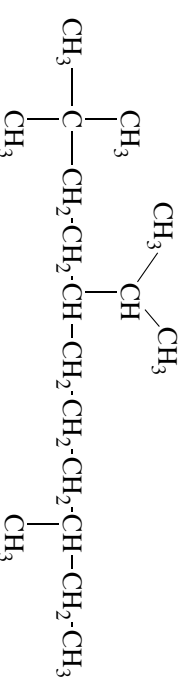
- 2) If Structure Contains a Ring That Has More Carbon Atoms Than Any Other Open Chain, the Main Chain is the Ring and is Named by Adding cyclo to the Name of the Alkane with the Same Number of Carbon Atoms as the Ring. The Rest is the Same as for Normal Alkane Except You Need to Keep the Total Numbers as Small as Possible When Numbering.

Ex. 1,2-dimethylcyclohexane

- 3) If More Than One Branch, List Them in Alphabetical Order, NOT Numerical Order.
Ex. 5-ethyl-3,4-diisopropyl-7-methyldecane

- 4) DO NOT Include the Italicized Prefixes *n*-, *sec*-, and *tert*- OR the Multiplying Prefixes *di*-, *tri*-, *tetra*-, etc. When Alphabetizing Simple Substituents. All Other Prefixes (*iso*-, *neo*-, etc.) are Included When Alphabetizing Simple Substituents. No Need to Argue, I Did Not Invent These Rules!
Ex. 5-*tert*-butyl-2-methyldecane

Big Old Hairy Example:



5-Isopropyl-2,2,9-trimethylundecane

What you need to know

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

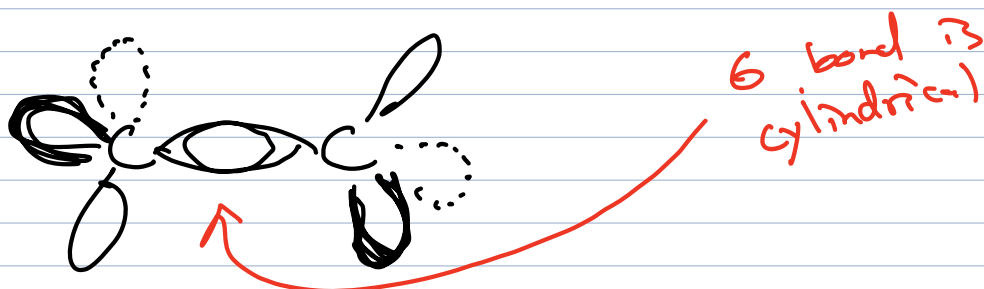
A molecule with higher energy is less stable

A molecule with lower energy is more stable

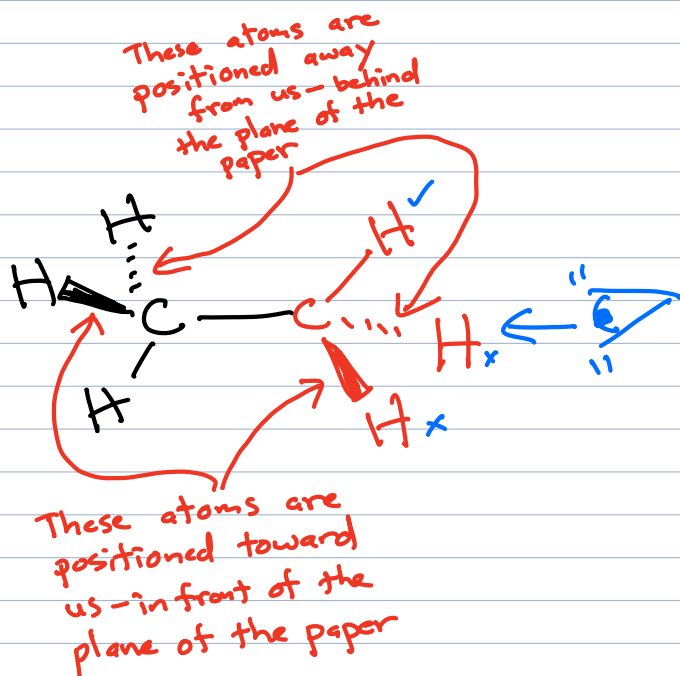
Strain in molecules raises energy and decreases stability

⇒ Molecules are found predominantly in their lowest energy (most stable) form.

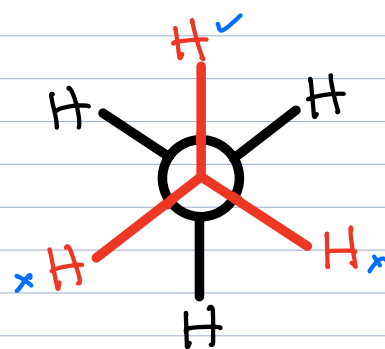
Carbon-Carbon sigma bonds rotate rapidly at room temperature



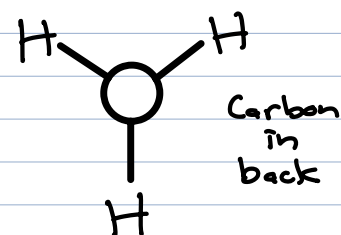
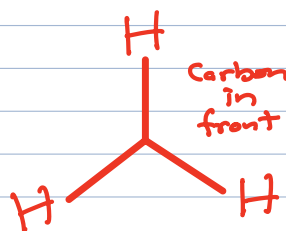
It does not get weaker as the bond rotates



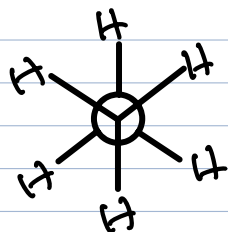
Newman Projection



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



Two extremes



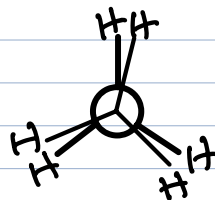
Staggered
Conformation



More stable



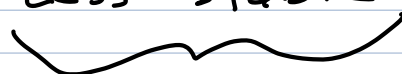
minimal torsional
strain



Eclipsed
Conformation



Less stable



torsional strain
is present

Torsional Strain \rightarrow a complex effect that
is based upon

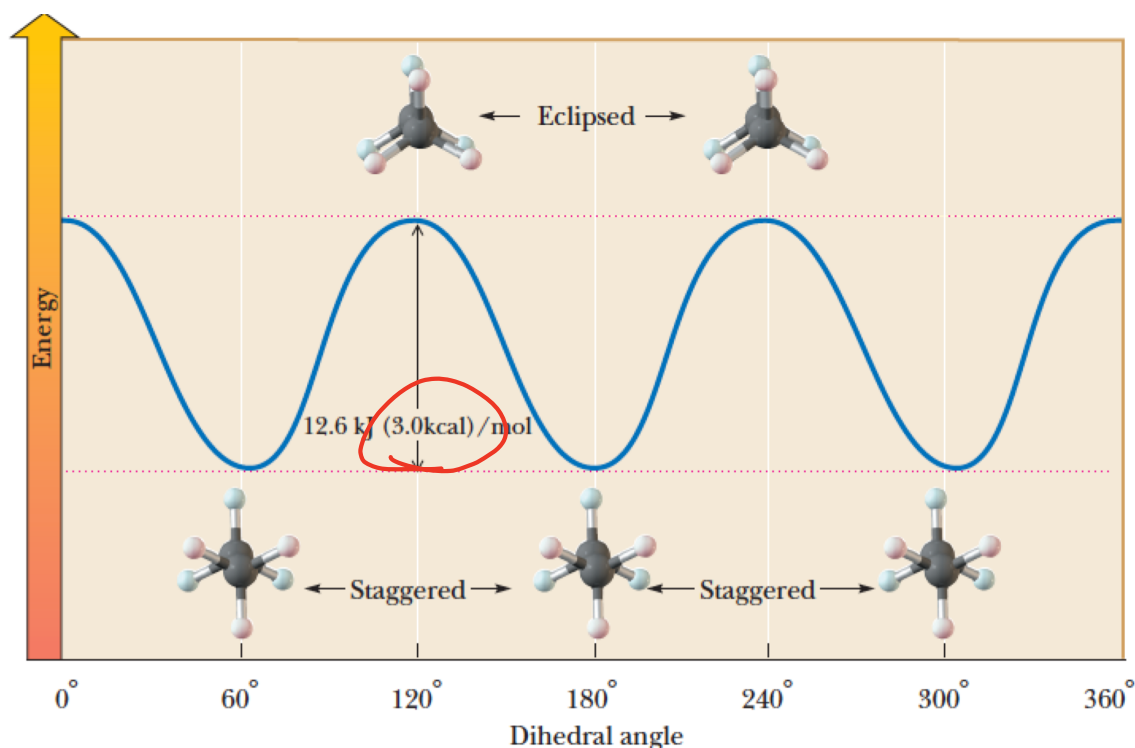
TIME CAPSULE



we will discuss
hyperconjugation
in chapter 6

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

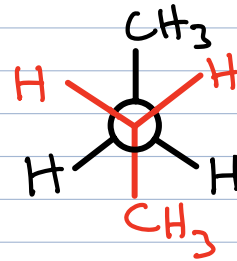
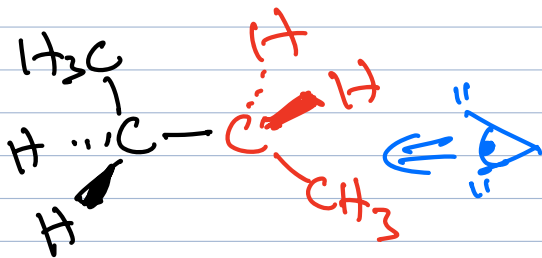
The ethane molecule rotates freely at room temperature, but because of torsional strain, it spends most of its time in the staggered conformation



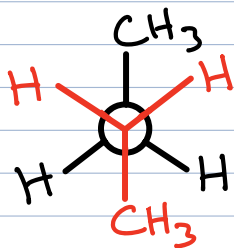
New type of strain \Rightarrow important for
alkanes of 4 or more
carbon atoms

Steric strain \rightarrow strain that is caused when
atoms "crunch" into each
other.

Butane \rightarrow 4 carbon atoms \rightarrow 3
different staggered conformations
 \Rightarrow These differ in energy



3 different staggered conformations

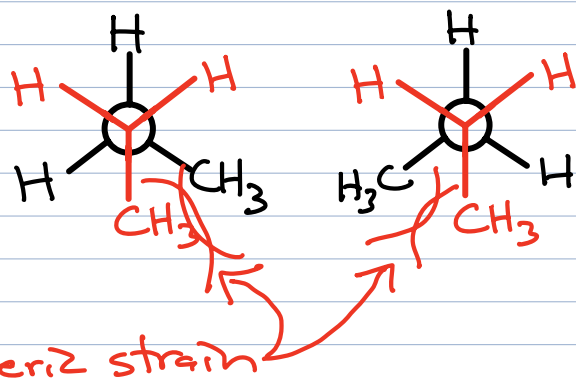


Anti

(methyl groups are as far apart as possible)

No steric strain

Lower in energy



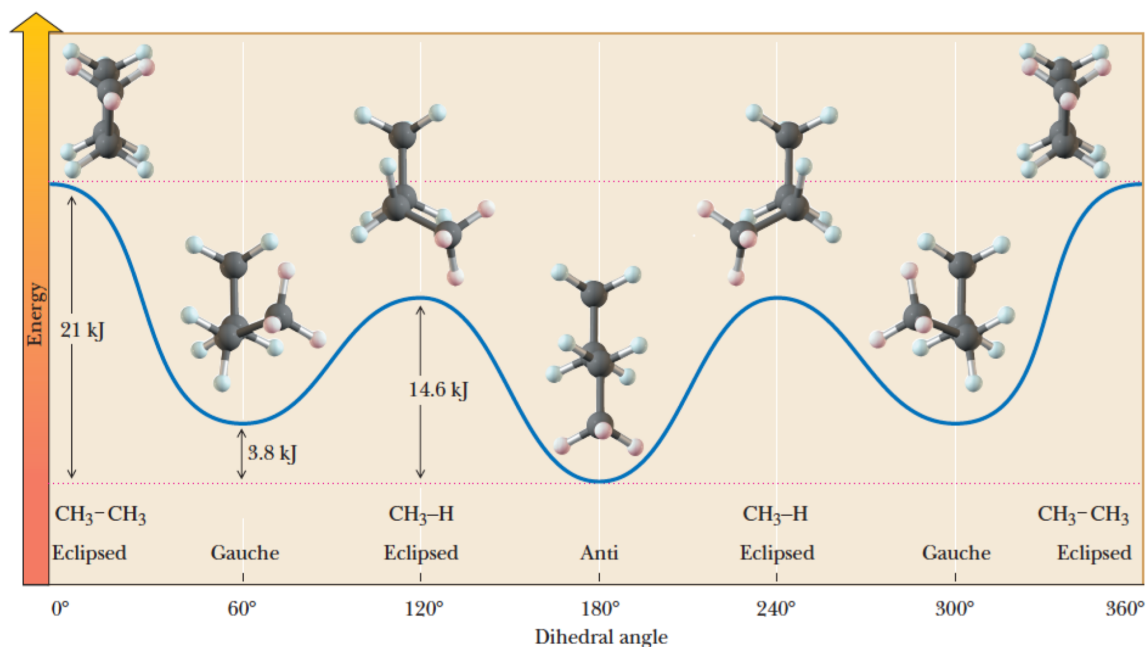
Steric strain

Gauche

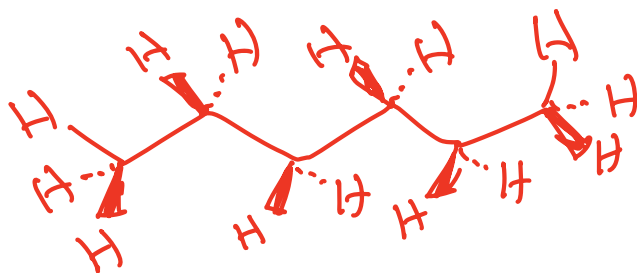
(methyl groups are adjacent)

Steric strain is present because the methyl groups "crunch" into each other

Higher in 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 amplitude of bond vibrations to increase

Very disorganized bond rotation \rightarrow 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
torsional strain

Cyclobutane

↓
Highly Strained



Angle and
torsional
strain

Not flat

"Puckers"
to relieve
some strain

Cyclopentane

"Puckers" to create
an "envelope"
conformation



Very little strain

Little angle strain
but some torsional
strain

Cyclohexane \rightarrow most stable cyclohexane

\rightarrow Adopts a chair conformation



Minimal
angle
strain



No torsional
strain

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

\Rightarrow "Keep it parallel"

