

## 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

Yes, Branch Has  
Branches Of Its Own

- 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 .

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

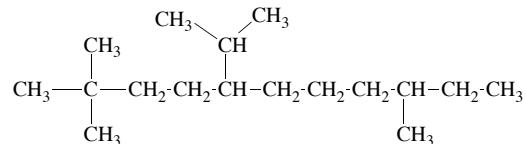
3) If More Than One Branch, List Them in Alphabetical Order, NOT Numerical Order.

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

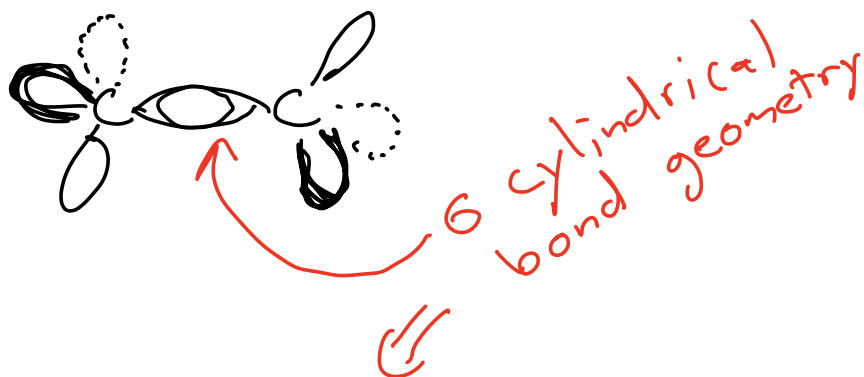
A molecule with higher energy is less stable

A molecule with lower energy is more stable

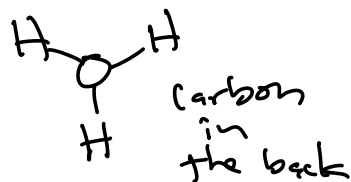
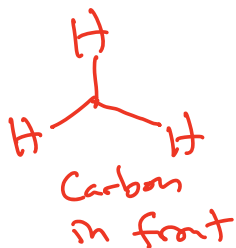
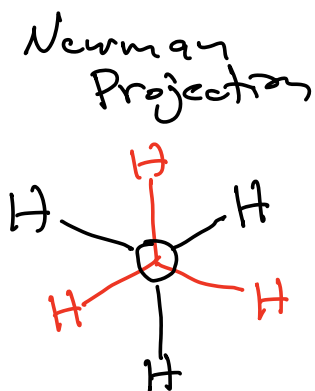
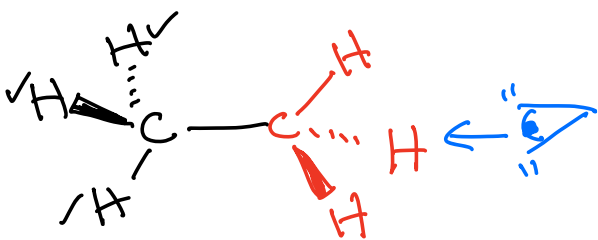
Strain in molecules raises energy and decreases stability

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

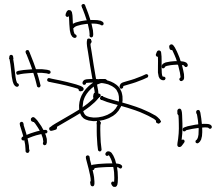
Carbon-Carbon sigma bonds rotate rapidly at room temperature



It does not get weaker as the bond rotates



Two extremes



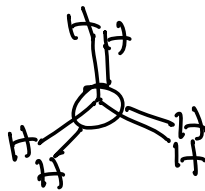
Staggered  
Conformation



More stable



Minimal torsional  
strain



Eclipsed  
Conformation



Less stable



Torsional  
Strain is  
present

Torsional Strain → a complex effect  
based on

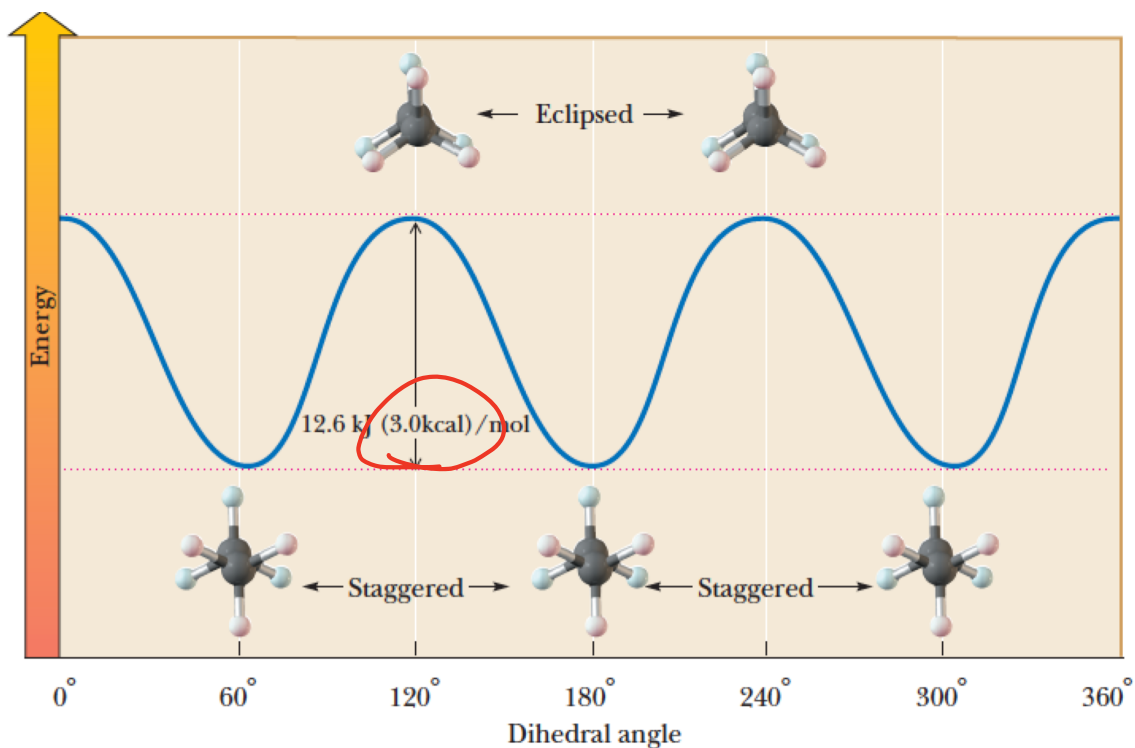
TIME  
CAPSULE



We will discuss  
in Chpt. 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

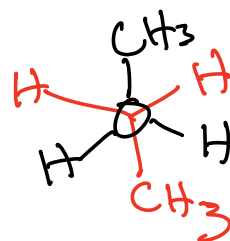
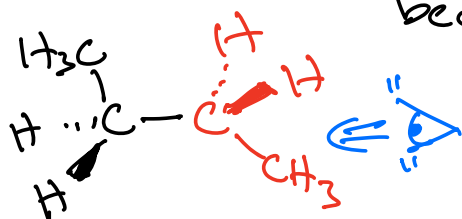
Steric strain  $\rightarrow$  strain caused when  
when atoms "crunch"  
into each other

Butane  $\rightarrow$  4 carbon atoms

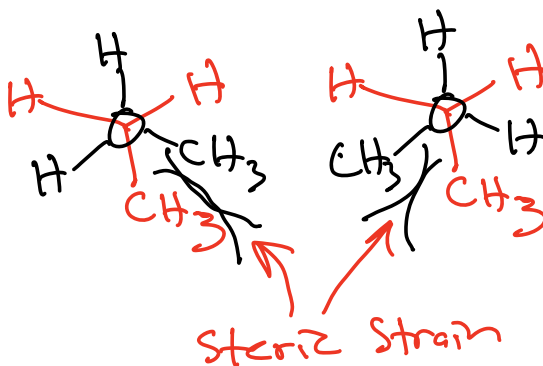
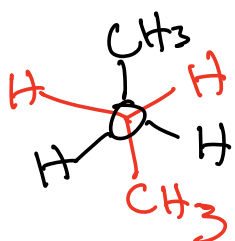
$\rightarrow$  3 different staggered conformations

$\Rightarrow$  These differ in energy

because of steric strain



3 different staggered conformations



Anti

(methyl groups are as far apart as possible)

No steric strain

Lower energy

Gauche

(methyl groups are adjacent)

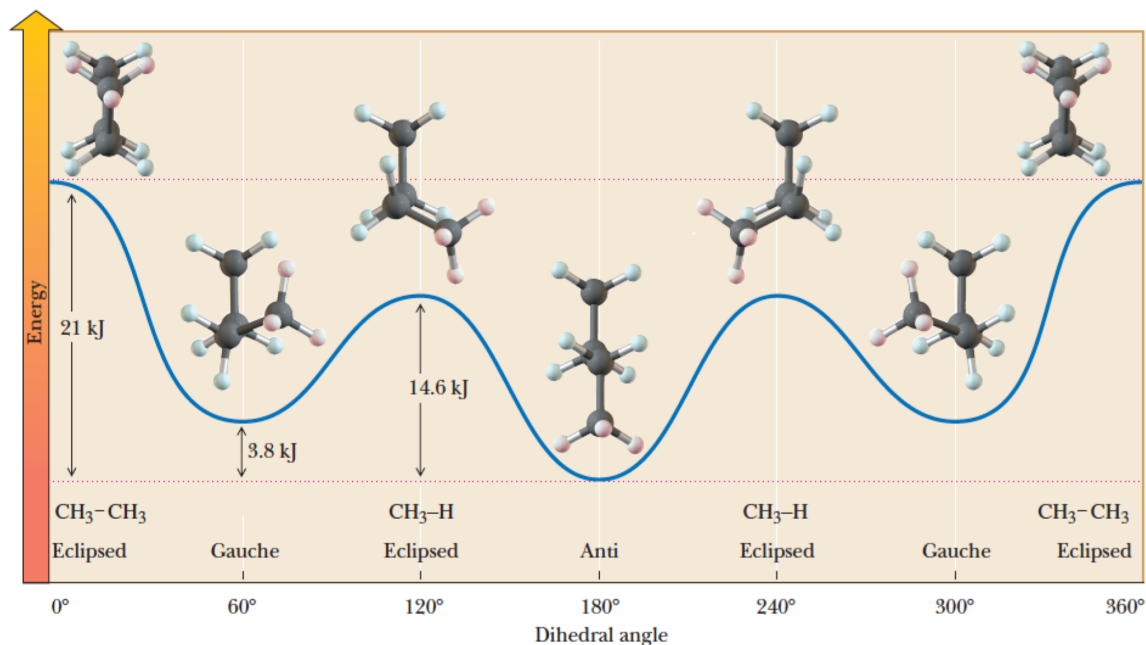
Steric strain

because poor

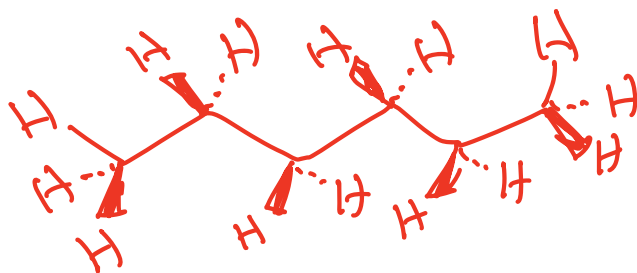
methyl groups

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





Dynamics  $\rightarrow$  heat in molecules causes 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  $109.5^\circ$

$\rightarrow$  Happens in ring structures

# Cycloalkanes

Cyclopropane

↓  
Highly Strained



High angle strain  
and  
torsional strain

Cyclobutane

↓  
Highly Strained



Not flat

Angle and  
torsional  
strain

"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"

