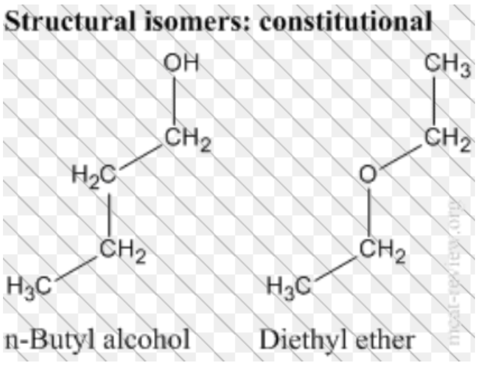
Some beginning vocab for naming:

Alkane (C_nH_{2n+2})

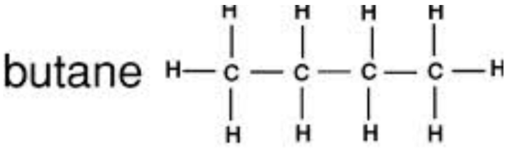


Cycloalkane (C_nH_{2n})

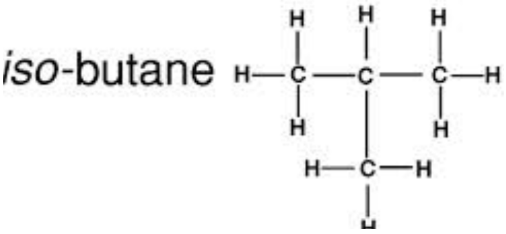
Alkene (C_nH_{2n})

Alkyne (C_nH_{2n-2})

Hydrocarbon



Consitutional isomers



Straight chain vs branched chain

Chains of alkanes- naming and properties:

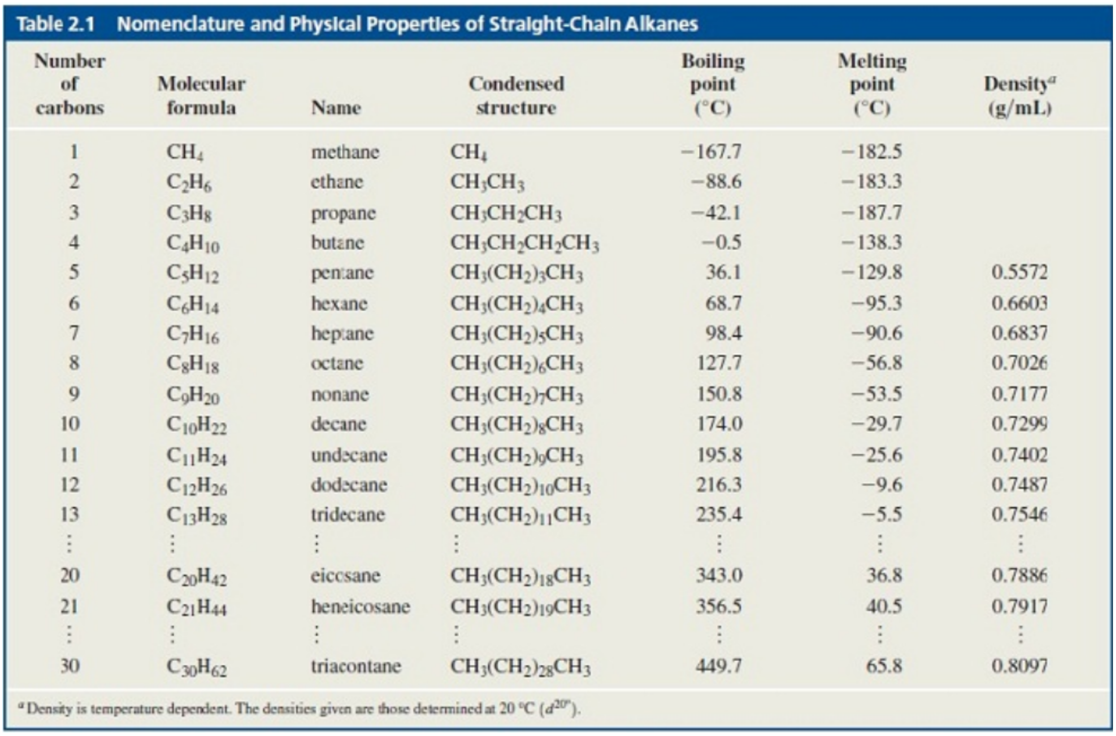


Table 2.1 Nomenclature and Physical Properties of Straight-Chain Alkanes

Number of carbons	Molecular formula	Name	Condensed structure	Boiling point (°C)	Melting point (°C)	Density[a] (g/mL)
1	CH_4	methane	CH_4	−167.7	−182.5	
2	C_2H_6	ethane	CH_3CH_3	−88.6	−183.3	
3	C_3H_8	propane	$CH_3CH_2CH_3$	−42.1	−187.7	
4	C_4H_{10}	butane	$CH_3CH_2CH_2CH_3$	−0.5	−138.3	
5	C_5H_{12}	pentane	$CH_3(CH_2)_3CH_3$	36.1	−129.8	0.5572
6	C_6H_{14}	hexane	$CH_3(CH_2)_4CH_3$	68.7	−95.3	0.6603
7	C_7H_{16}	heptane	$CH_3(CH_2)_5CH_3$	98.4	−90.6	0.6837
8	C_8H_{18}	octane	$CH_3(CH_2)_6CH_3$	127.7	−56.8	0.7026
9	C_9H_{20}	nonane	$CH_3(CH_2)_7CH_3$	150.8	−53.5	0.7177
10	$C_{10}H_{22}$	decane	$CH_3(CH_2)_8CH_3$	174.0	−29.7	0.7299
11	$C_{11}H_{24}$	undecane	$CH_3(CH_2)_9CH_3$	195.8	−25.6	0.7402
12	$C_{12}H_{26}$	dodecane	$CH_3(CH_2)_{10}CH_3$	216.3	−9.6	0.7487
13	$C_{13}H_{28}$	tridecane	$CH_3(CH_2)_{11}CH_3$	235.4	−5.5	0.7546
⋮	⋮	⋮	⋮	⋮	⋮	⋮
20	$C_{20}H_{42}$	eicosane	$CH_3(CH_2)_{18}CH_3$	343.0	36.8	0.7886
21	$C_{21}H_{44}$	heneicosane	$CH_3(CH_2)_{19}CH_3$	356.5	40.5	0.7917
⋮	⋮	⋮	⋮	⋮	⋮	⋮
30	$C_{30}H_{62}$	triacontane	$CH_3(CH_2)_{28}CH_3$	449.7	65.8	0.8097

[a] Density is temperature dependent. The densities given are those determined at 20 °C ($d^{20°}$).

As Carbon chain lengthens, what happens to:

MP

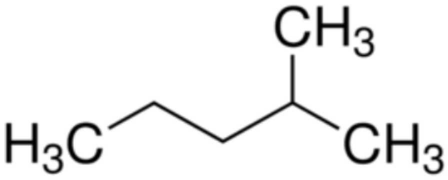
BP

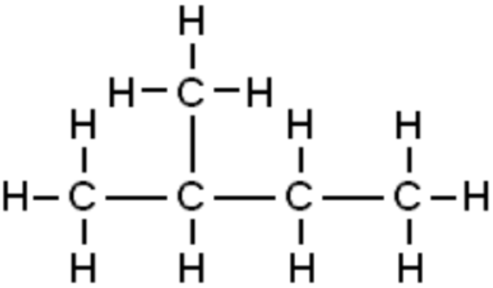
Density

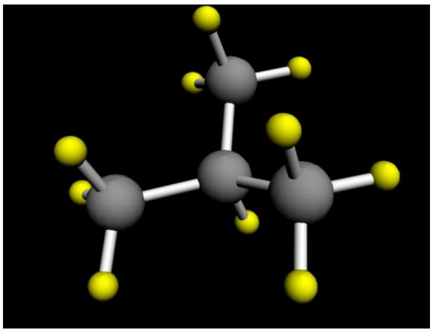
WHY???

Some units and basic "common" names to know:

"iso" prefix - C bonded to a H and 2 other CH_3 groups







Common Names of some things - match them to their picture

Isobutane Isopentane Isohexane

The Systematic IUPAC Nomenclature of Alkanes:

1) Determine the number of carbons in the longest chain

2) Number the chain in the direction that gives the substituent the lower number

3) Numbers are used only for systemic names, never for common names

4) Substituents are listed in alphabetical order

5) A number and a word are separated by a hyphen; numbers are separated by a comma

6) ***Di, tri, tetra, sec,*** and ***tert*** are ignored in alphabetizing

7) ***Iso*** and ***cyclo*** are **not** ignored in alphabetizing (when they are a branch)

8) Only if the same set of numbers is obtained in both directions does the first group stated get the lowest number

9) In the case of two hydrocarbon chains with the same number of carbons, choose the one with the most substituents

10) If there is only one substituent on the ring of a cycloalkane, do not give that substituent a number

11.) When main structure is a cyclic structure - cyclo______ is part of the main alkanes name. Additional branches may be added before as in chain alkanes.

Naming of branches:

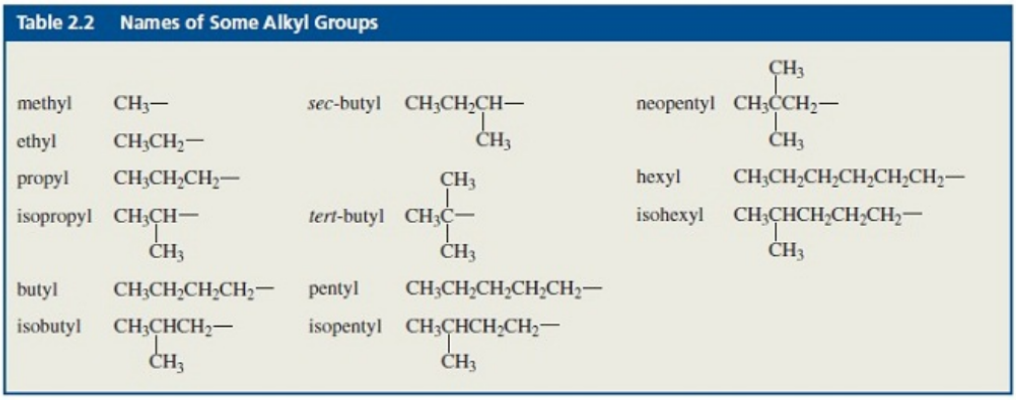


Table 2.2 Names of Some Alkyl Groups

methyl	$CH_3—$	*sec*-butyl	$CH_3CH_2\underset{CH_3}{\underset{\mid}{C}}H—$	neopentyl	$CH_3\overset{CH_3}{\overset{\mid}{\underset{CH_3}{\underset{\mid}{C}}}}CH_2—$
ethyl	$CH_3CH_2—$				
propyl	$CH_3CH_2CH_2—$			hexyl	$CH_3CH_2CH_2CH_2CH_2CH_2—$
isopropyl	$CH_3\underset{CH_3}{\underset{\mid}{C}}H—$	*tert*-butyl	$CH_3\overset{CH_3}{\overset{\mid}{\underset{CH_3}{\underset{\mid}{C}}}}—$	isohexyl	$CH_3\underset{CH_3}{\underset{\mid}{C}}HCH_2CH_2CH_2—$
butyl	$CH_3CH_2CH_2CH_2—$	pentyl	$CH_3CH_2CH_2CH_2CH_2—$		
isobutyl	$CH_3\underset{CH_3}{\underset{\mid}{C}}HCH_2—$	isopentyl	$CH_3\underset{CH_3}{\underset{\mid}{C}}HCH_2CH_2—$		

Br -

Cl -

F -

I -

Some notes about use of these branches:

1.) "sec" - used with butyl - using it with a longer chain is not true, there is more than 1 "sec" C

2.) Compounds have common names and IUPAC names (red = common, blue = IUPAC in our book)

DO NOT USE NUMBERS WITH COMMON NAMES

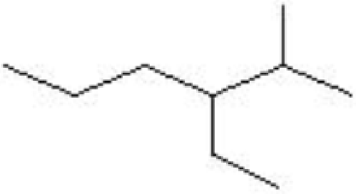
Skeletal Structures:

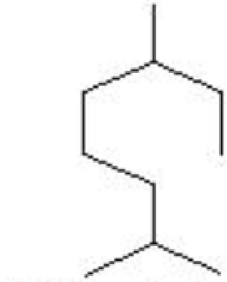
- Do not show any C or H
- If any other atoms are present, they are shown
- Structures are neutral unless a formal charge is shown.

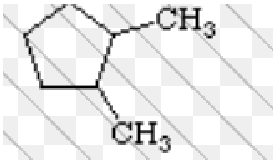
How many bonds vs attached H are needed per:

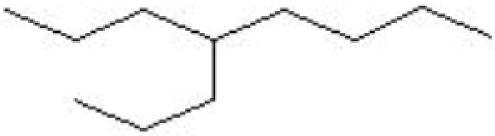
C N O

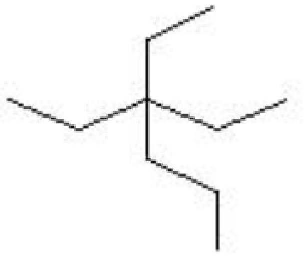
Practice:

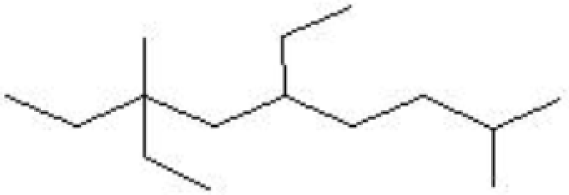


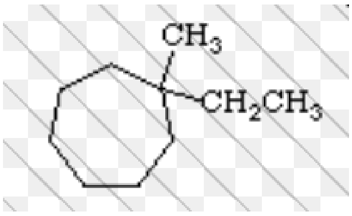


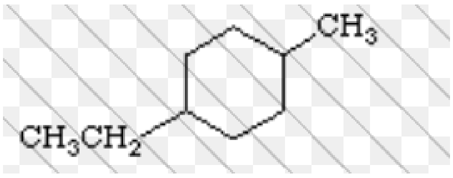


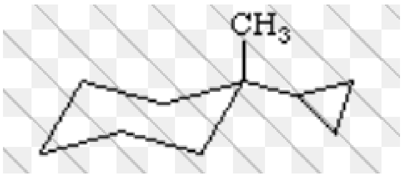






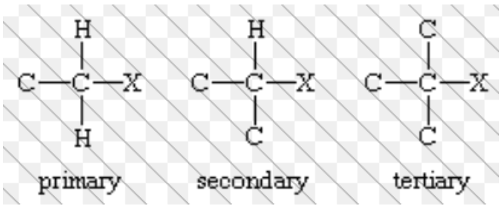

CH3
CH2CH3


CH3
CH3CH2


CH3

Classifying and naming alkyl halides, alcohols, and amines:

For Alchohol and Alkyl halides:



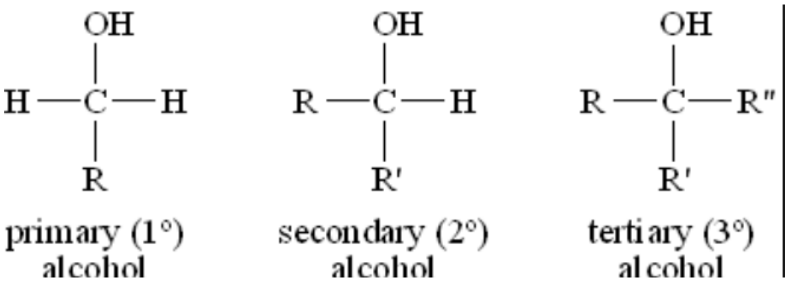
Alkyl halides

- See what C the branch is on

Primary

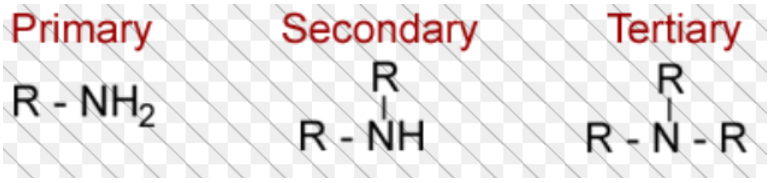
Secondary

Tertiary



For Amines:

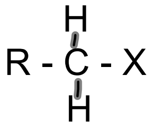
- Primary, secondary and tertiary refers to how many C are bonded to Amine



Review of Hybridization:

sp^3 hybridization for:

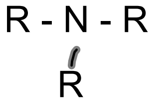
Halogens to carbon chain



$$\mathrm{R}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\mathrm{X}$$

Oxygen when 2 single bonds R - C - O - C - R

Nitrogen with 3 bonds



$$\mathrm{R}-\underset{\mathrm{R}}{\mathrm{N}}-\mathrm{R}$$

IYSICAL PROPERTIES:

1) **Boiling Points:** - for each, determine intermolecular force present and describe the trend in boiling points for each functional group

a) Alkanes:

b) Alkyl Halides:

c) Alcohols:

d) Amines:

2) **Melting points:**

3) **Solubility:**

a) Alkanes:

b) Alcohols:

c) ethers:

d) Amines:

e) Halides:

Rotation around C - C single bonds:

a.) sp3 - sp3 bonding

b.) Conformations - Spatial arrangements of atoms due to rotation around a single bond

c.) Newman projections - Drawings along longitudinal axis of C - C bond

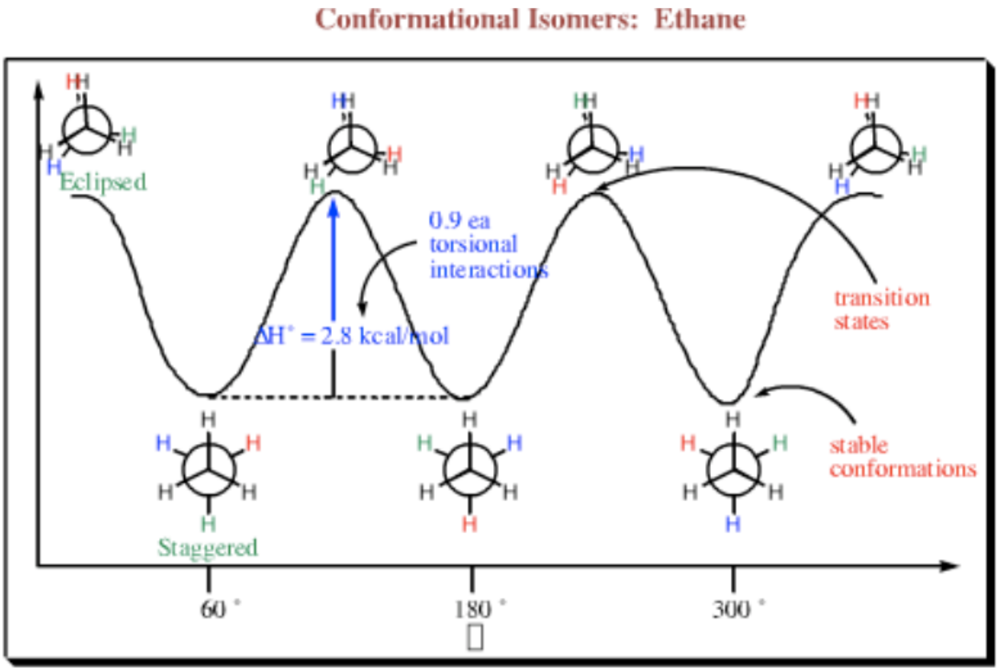
O = back C ⅄ = front C — = attachments to each C

Ethane: CH_3CH_3

Staggered -

Eclipsed -

Graph of energy at different conformations of ethane:



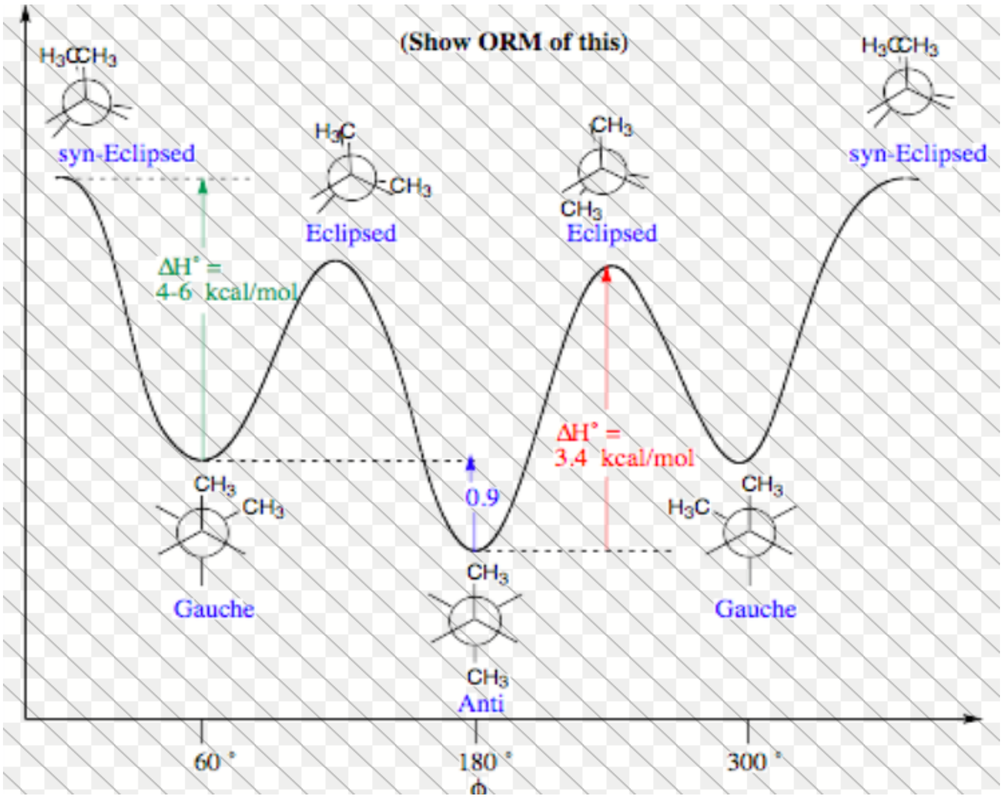
Butane Conformations: CH_3 - CH_2 - CH_3

a.) Now have 2 bonds to rotate around

b.) Forms 3 staggered, 3 eclipsed conformations

Best option - when CH3 groups are as far apart as possible

Worst option - when CH3 groups are closest

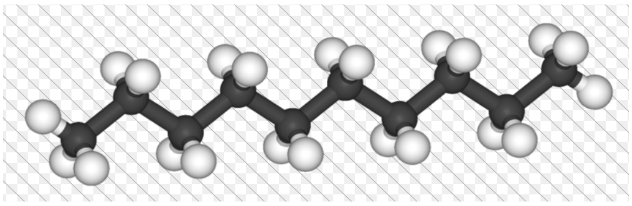


Steric strain- strain experienced by atom or mlecules from being too close and having repulsion occur

- as the repelling groups get larger in size this = more steric strain

** More stable the conformation = more time the molecule spends in it

**This is what causes long chains to form the zig-zag appearance



Cycloalkanes and angle strain:

a.) **Angle strain -** deviation of cyclo angle from the expected value

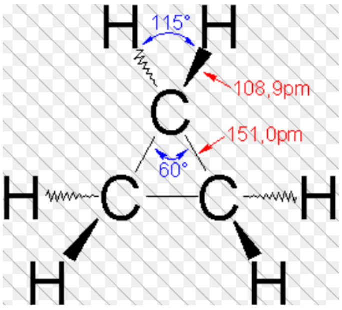
b.) Most cyclic structures are 5-6 carbons - we assume this must be more stable than having more or less C

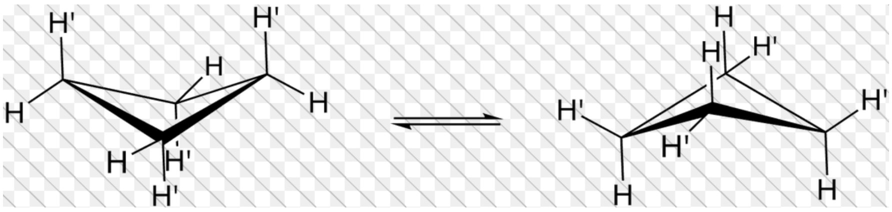
c.) Carbons in a cyclic structure = sp3

d.) Some cyclic structures with angle strain

cyclobutane = less than 90^0

cyclopropane = 60^0





Cyclohexane:

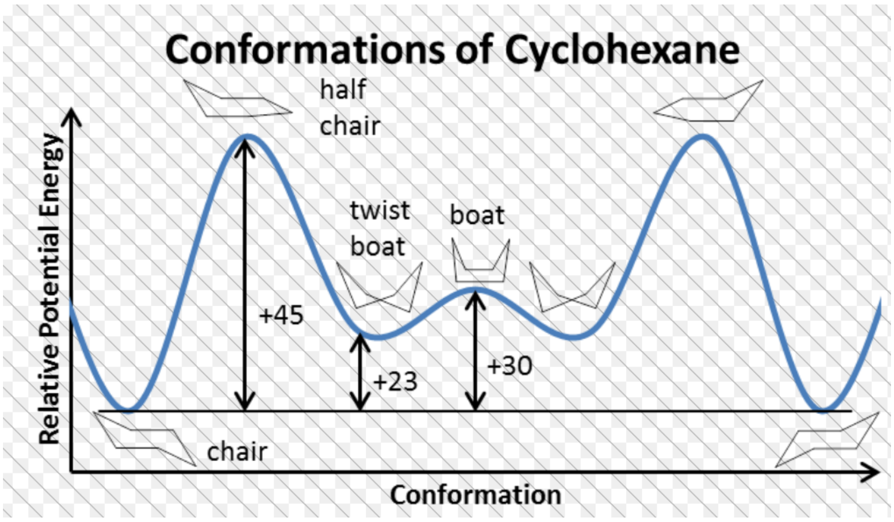
a.) 6 - C cyclic ring

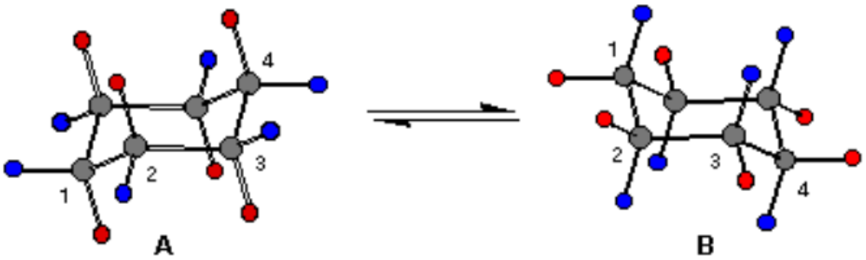
b.) Has several conformations, having varying energy levels and stabilities

c.) Chair formation = most stable - there are 2 chair formations

*** Cyclohexane **ring flips** 10^5 per second between these formations

*** A rotation flip between chair conformations is called a **Ring flip**





Notice what happens to all axial and equatorial as the ring flip occurs

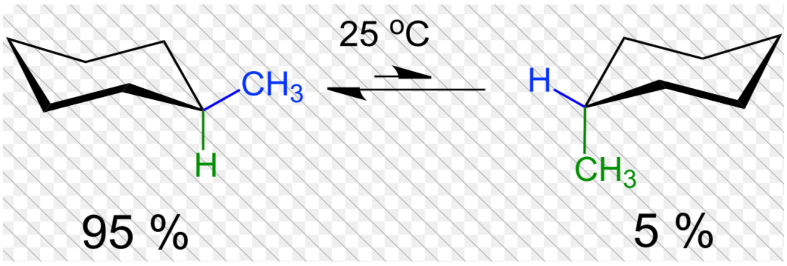
Substituted cyclohexane conformations:

Monosubstituted:

- 1 substituent on the cyclohexane ring

- most stable if the substituent is in the equatorial position of chair conformation

WHY??



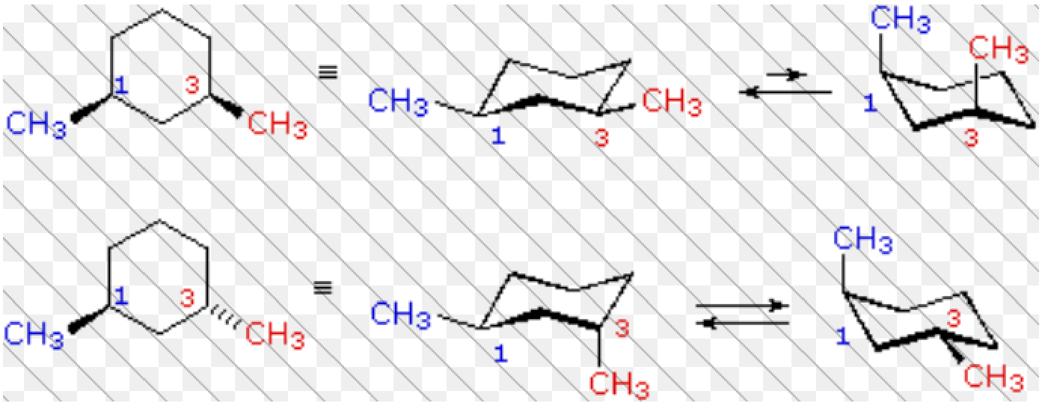
Disubstituted:

- 2 substituents on cyclohexane ring

2 isomers are possible:

a.) Cis - having substituents on same side of the ring

b.) Trans -having the substituents on opposite sides of the ring



Notice:

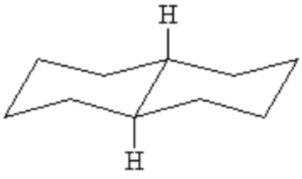
a.) Even after ring flip the branches are still cis and trans, ring flip DOES NOT change them from being a cis or trans compound

b.) When are they in their most stable positions?

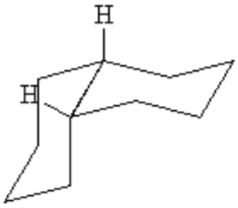
c.) If their is not a cis or trans that puts both substituents equatorial, the largest substituent should be equatorial

<u>Fused cyclohexanes:</u>

- when 2 cyclohexane rings are fused
- may be cis or trans isomers
    - * trans is more stable = less energy



trans



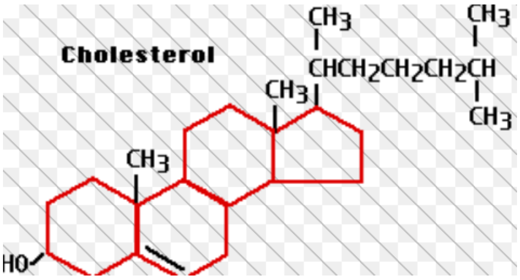
cis

Hormones: chemical messengers delivered in blood stream to target area, then stimulate or inhibit the process

ex: cholesterol = a steroid - often a precursor to other steroids

Pg 80- Cholesterol and heart disease

a.) Body makes cholesterol, too much =



b.) 2 types of cholesterol:

c.) What does eating too much cholesterol do to our normal levels of each cholesterol?

d.) Clinical treatment of high cholesterol:

1) Angle strain: the strain due to expansion or compression of bond angles

2) Torsional strain: the strain due to eclipsing of neighboring bonds

3) Steric strain: the strain due to repulsive interactions when atoms approach each other too closely

Cycloalkane	Ring size	Heat of Comb. kcal/mol	Ht of comb/CH_2 kcal/mol	total strain kcal/mol
cyclopropane	3	499.8	166.6	27.6
cyclobutane	4	655.9	164.0	26.4
cyclopentane	5	793.5	158.7	6.5
cyclohexane	6	944.5	157.4	0
cycloheptane	7	1108	158.4	6.3
cyclooctane	8	1269	158.6	9.6
cyclononane	9	1429	158.8	12.6
cyclodecane	10	1586	158.6	12.0
cycloundecane	11	1742	158.4	11.0
cyclododecane	12	1891	157.6	2.4
cyclotridecane	13	2051	157.8	5.2
cyclotetradecane	14	2204	157.4	0
Alkane (reference)			157.4	

(A)Use dimethylcyclohexane:

cis/trans substitution pattern	axial/equatorial relationships
1,2 - cis disubstituted	
1,2 - trans disubstituted	
1,3 - cis disubstituted	
1,3 - trans disubstituted	
1,4 - cis disubstituted	
1,4 - trans disubstituted	

(B)Draw both chair forms and label which is the most stable conformation of

cis - 1 - tert-butyl - 4 - chlorocyclohexane