CH203 Lecture 6

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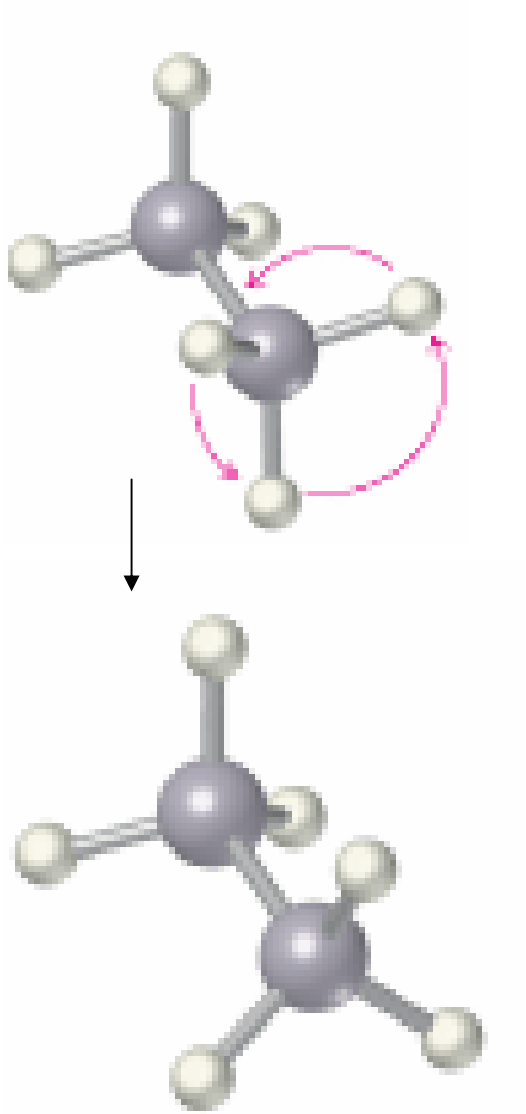
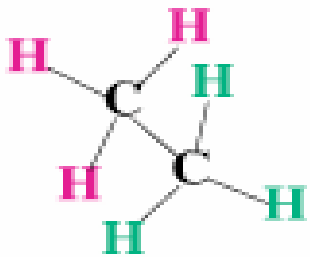
Conformations of Ethane

- Conformers interconvert rapidly and a structure is an average of conformers
- Molecular models are three dimensional objects that enable us to visualize conformers
- Representing three dimensional conformers in two dimensions is done with standard types of drawings

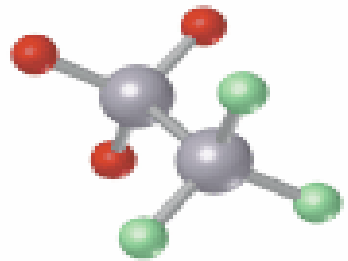


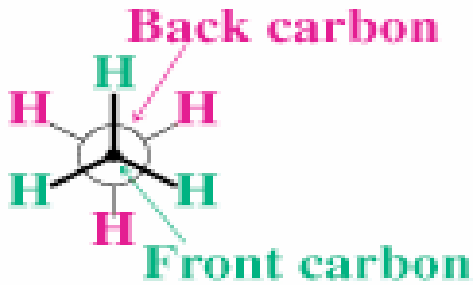
Representing Conformations

- **Sawhorse representations** show molecules at an angle, showing a molecular model
  - C-C bonds are at an angle to the edge of the page and all C-H bonds are shown
- **Newman projections** show how the C-C bond would project end-on onto the paper
  - Bonds to front carbon are lines going to the center
  - Bonds to rear carbon are lines going to the edge of the circle

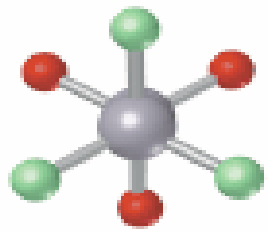


Sawhorse representation



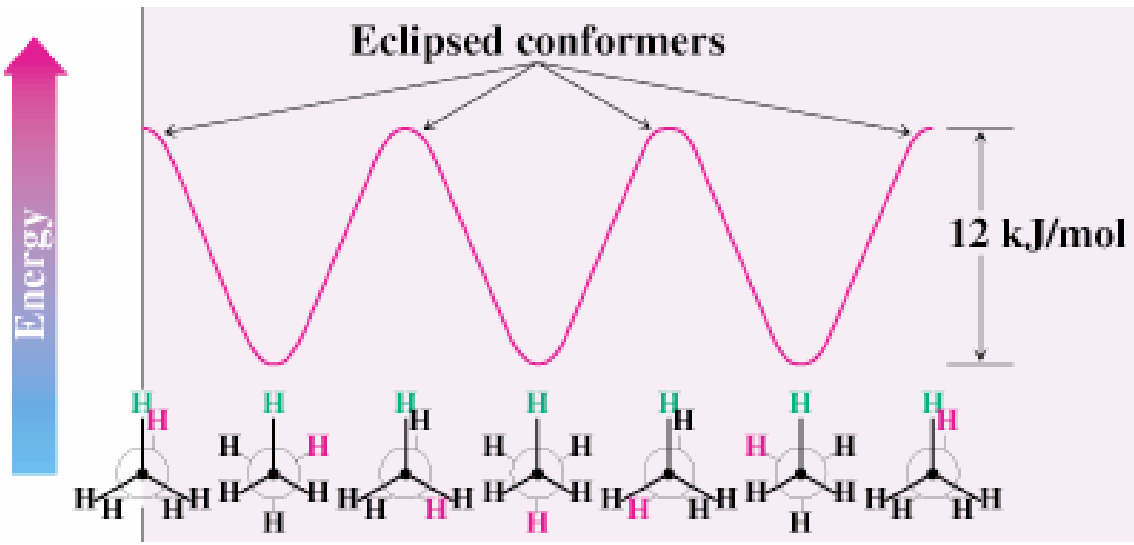


Newman projection



Ethane's Conformations

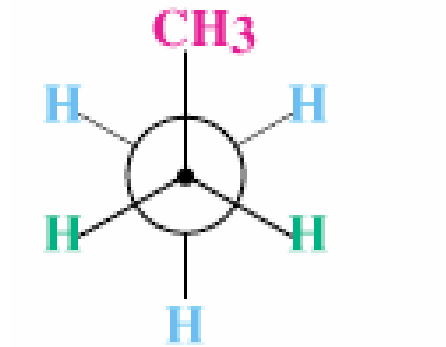
- There barrier to rotation between conformations is small (12 kJ/mol; 2.9 kcal/mol) The most stable conformation of ethane has all six C–H bonds away from each other (**staggered**)
- The least stable conformation has all six C–H bonds as close as possible (**eclipsed**) in a Newman projection – energy due to torsional strain



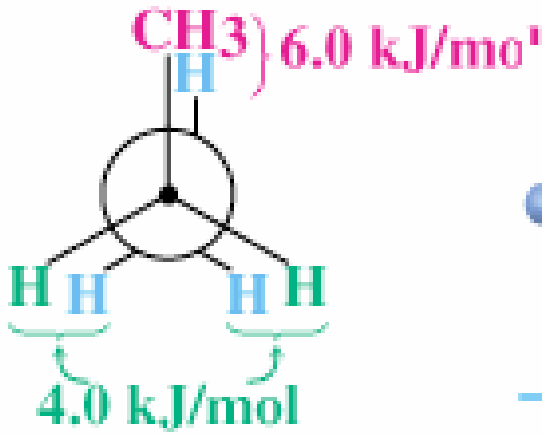
or 2.9 kcal/mol

Conformations of Propane

- Propane (C_3H_8) torsional barrier around the carbon–carbon bonds 14 kJ/mol
- Eclipsed conformer of propane has two ethane-type H–H interactions and an interaction between C–H and C–C bond



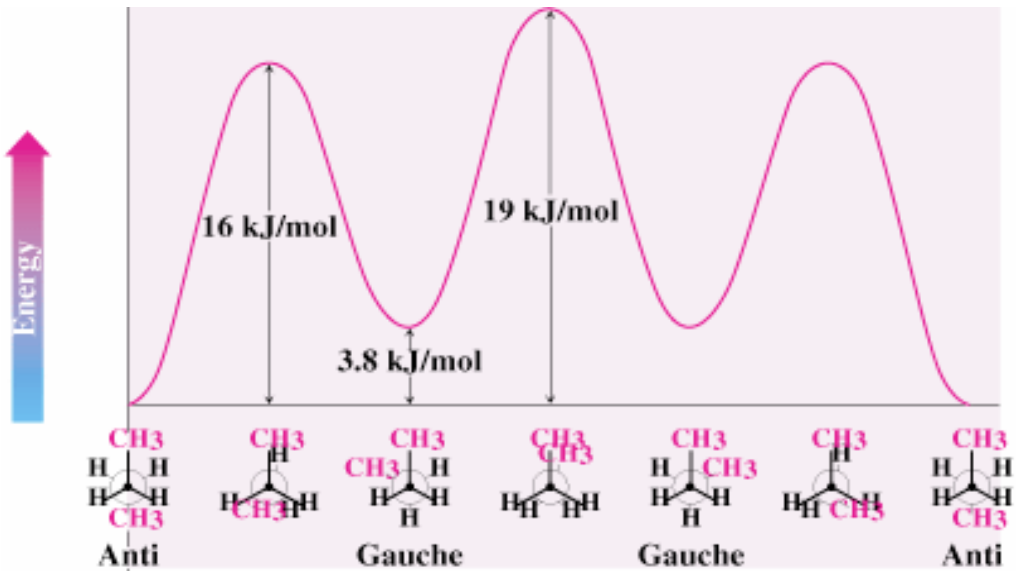
Staggered propane

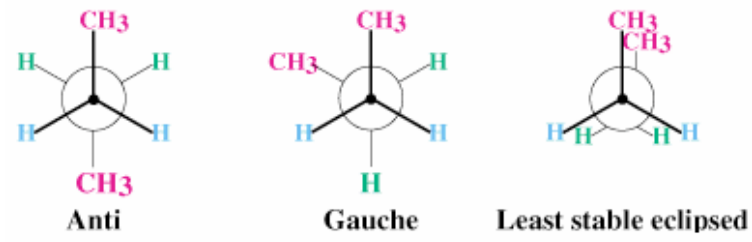


Eclipsed propane

Conformations of Butane

- **Anti conformation** has two methyl groups 180° away from each other
- Rotation around the C2–C3 gives eclipsed conformation
- Staggered conformation with methyl groups 60° apart is **gauche conformation**





Interaction Strain Energies

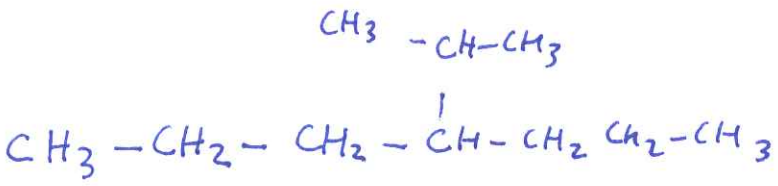
	[kcal/mol]
H,H eclipsed	1.0
CH_3,H eclipsed	1.4
CH_3,CH_3 eclipsed	2.6
CH_3,CH_3 *gauche*	0.9

Information will be provided for exams

CH 203 Lecture # 6

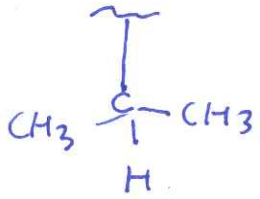
9/21/10

- Alkane naming handout on course website

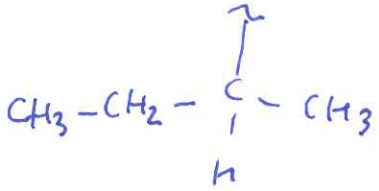


4-(1-methyl ethyl) heptane or 4-Isopropyl heptane

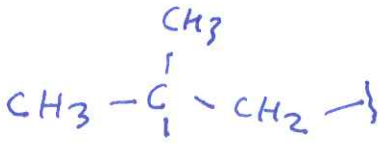
Can also use common names for branched chain alkyls



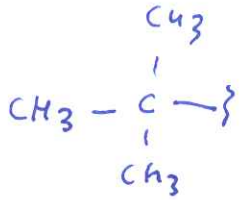
Isopropyl (i-Pr)



sec-butyl (sec-Bu)



Iso-butyl



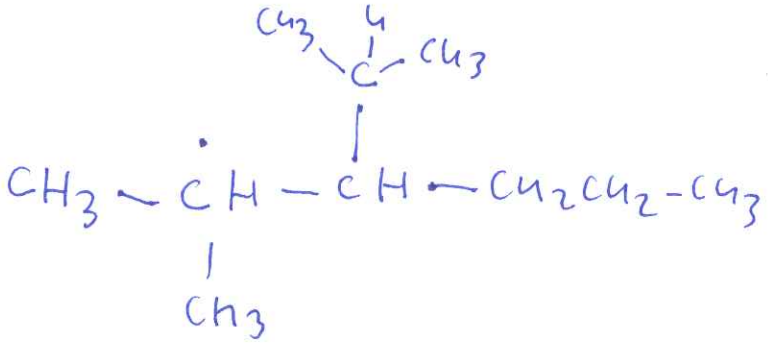
tert-butyl (t-Bu)

~~Lecture #16~~

Compound naming Ch. 3 p. 90

Isopropyl and Isobutyl are alphabetically listed under "i"

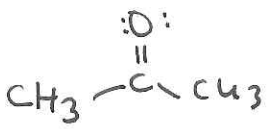
however sec-butyl and tert-butyl under "b"



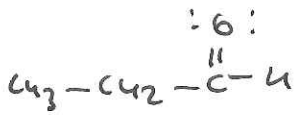
3-Isopropyl-2-methyl hexane

We have

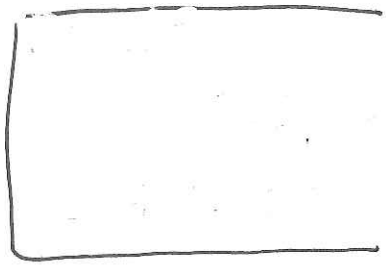
~~In Chapter 3,~~ learned about constitutional isomers:

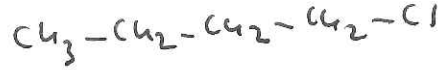


acetone

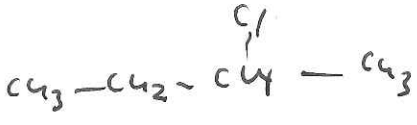


propionaldehyde





1-chlorobutane



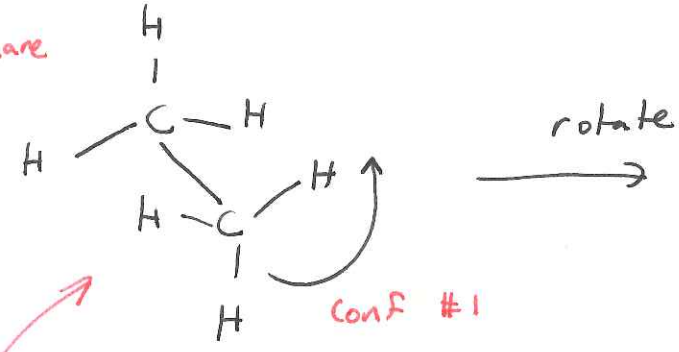
2-chlorobutane

In contrast, stereoisomers differ in the way atoms are arranged in 3D-space.

stereochemistry: branch of chem. that deals with spatial arrangements of atoms in molecules

Conformational isomers ~~are~~ result from different rotational arrangements of atoms ~~of~~ that can interconvert rapidly at rt.

ethane



Conformational isomers are also called conformers

Sawhorse representation: shows all C–H bonds

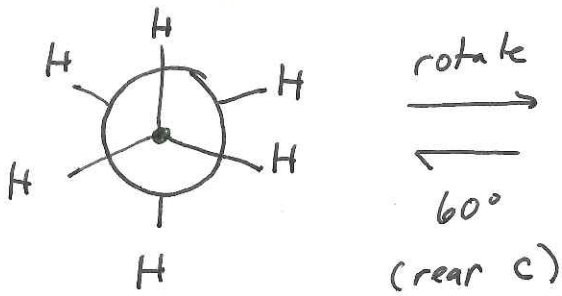
Newman projection : view the C–C bond directly end-on.

1 kcal = 4.1 kJ

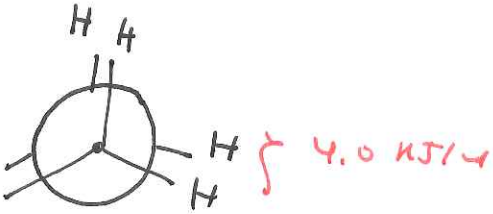
— Carbon in front represented by the point at which 3 bonds intersect

— Carbon in back represented by a circle.

conformations of ethane



~ 4.0 kJ/mol (1 kcal/mol)



~ 1%

"staggered conformation"

99%

most stable conformation : C–H bonds as far away from each other as possible

do not observe perfectly free rotation in ethane

"eclipsed conformation"

↳ least stable

C–H bonds very close (aligned)

"eclipsed"

Extra 12 kJ/mol (2.9 kcal/mol) present in eclipsed conf. of ethane is called

torsional strain : repulsion felt by bonding e⁻s of one C–H bond as they pass close to another C–H bond

one component of steric strain

- angle
- van der Waal's
- torsional
- ring

Conformational analysis : investigation of various conformations of a cpd + relative stabilities

[see attached overhead]

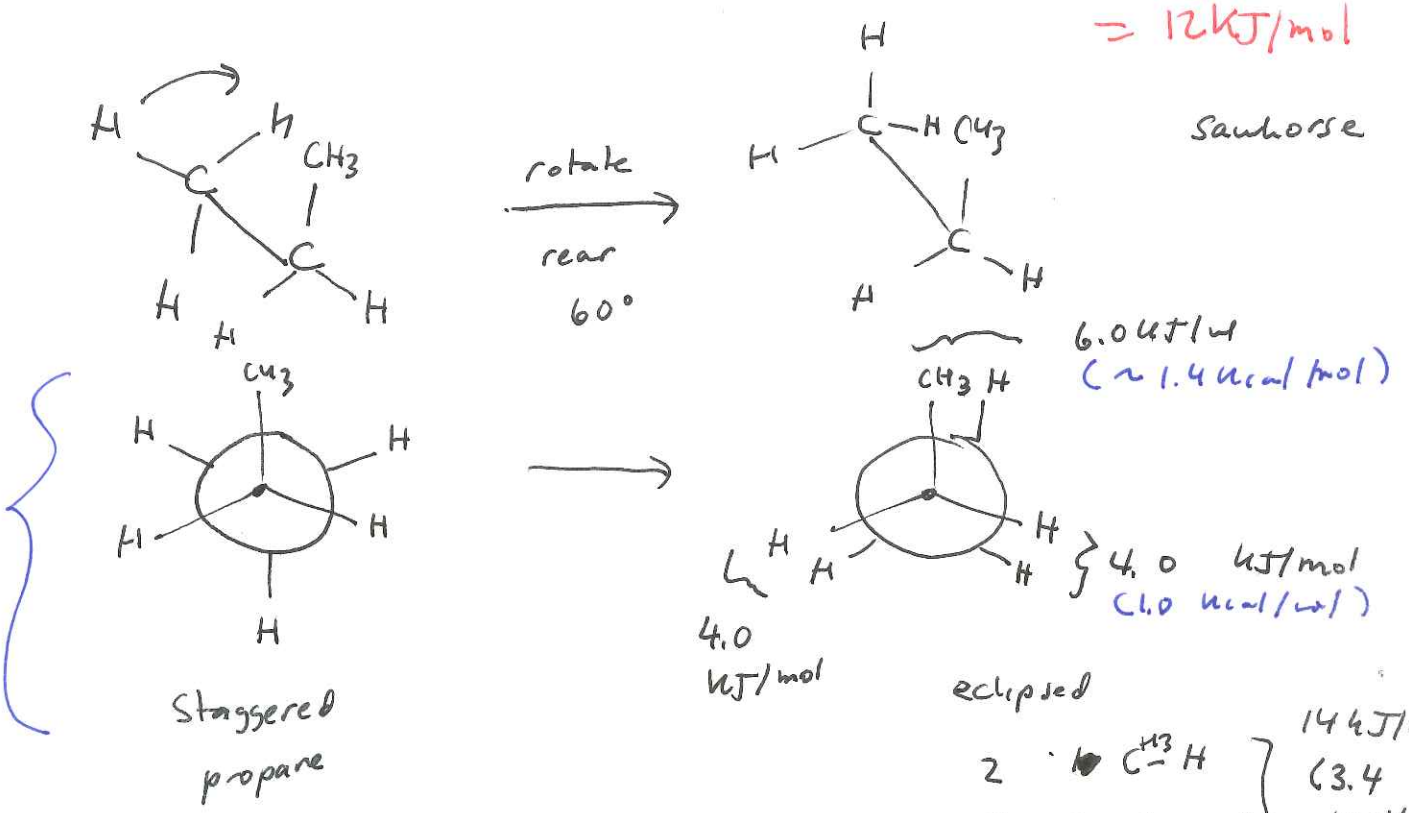
energy minimum : staggered

maximum : eclipsed

For ethane, the "barrier to rotation" of staggered to eclipsed conformers is ≈ 12 kJ/mol (2.9 kcal/mol)

≈ barrier to rotation around C–C single bond = 12 kJ/mol

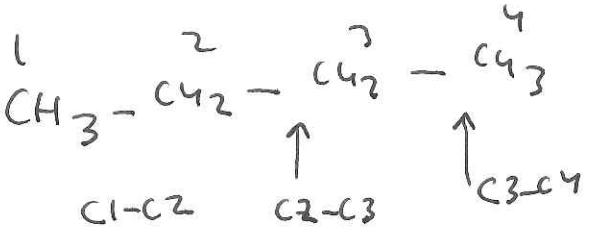
For propane:

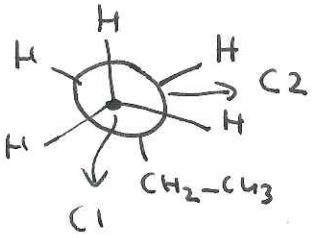


2 · H–CH3] 14 kJ/mol (3.4 kcal/mol)
1 C–C]

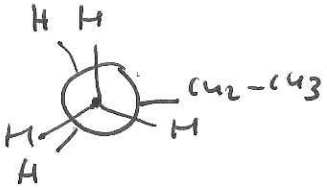
	kcal/mol
H–H eclipsed	1.0
CH3–H "	1.4

Butane has 3 – C–C single bonds and the molecule can rotate about each of them:





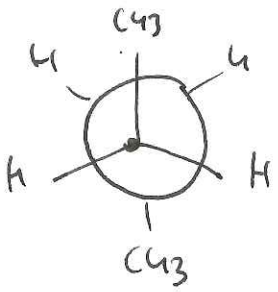
staggered conformation for rot about C1–C2 bond



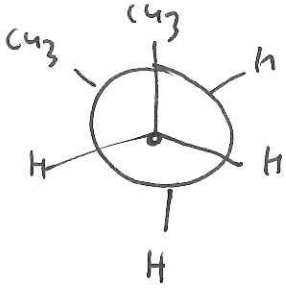
eclipsed conf for rot about C1–C2 bond

conformation

However, the staggered + eclipsed conformers resulting from rotation of the C2–C3 of butane do not have the same energy

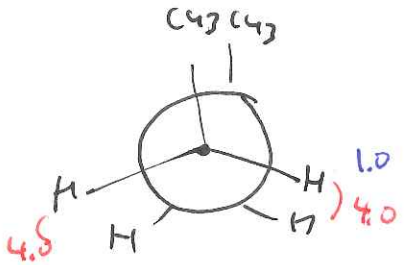


anti



gauche

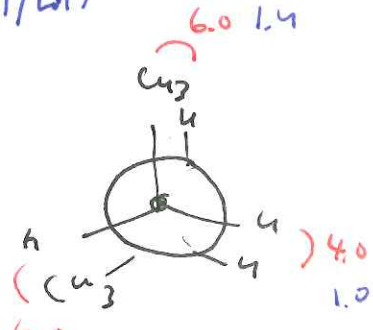
11 kJ/mol (2.6 kcal/mol)



(19 kJ/mol) 4.6 kcal/mol

least stable eclipsed

6.0 1.4



16 kJ/mol

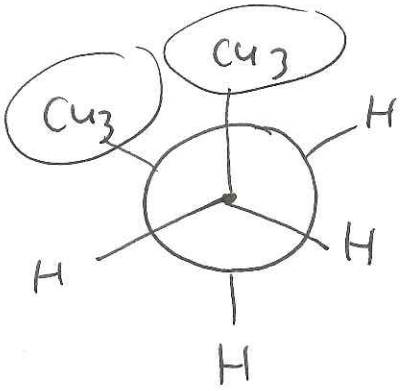
favored eclipsed

2 large –CH3 groups as far apart as possible

no torsional strain

energy maxima

Let's consider the special staggered conformations:



gauche conformation

3.8 kJ/mol

(0.9 kcal/mol)

higher than anti conformation

, even though it has no eclipsing interactions.

- Energy difference due to steric strain, repulsion between H atoms of the methyl groups (e^- clouds of C–H repel)

Useful to know energetic costs:

	kcal/mol
H ↔ H eclip	1.0
H ↔ CH_3 eclipsed	1.4
CH_3 ↔ CH_3 "	2.6
CH_3 ↔ CH_3 gauche	0.9

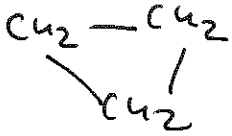
Chapter 4 : Organic Compounds: Cycloalkanes and Their Stereochemistry

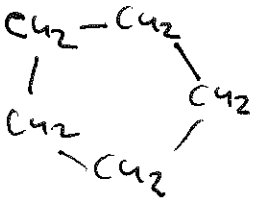
Assigned Problems 1, 2, 4, 5, 12, 13, 15, 18, 19, 33-35, 36, 37, 43-46, 49, 51, 55

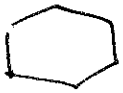
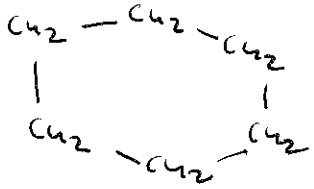
Cycloalkanes

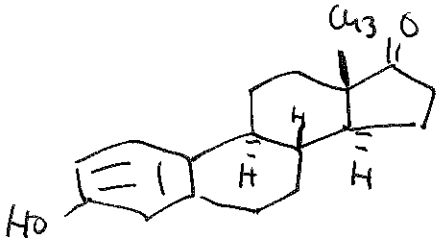
general formula $(CH_2)_n$

- attach prefix cyclo- to the names of alkanes possessing the same # of C atoms

 =  cyclopropane

 =  cyclopentane

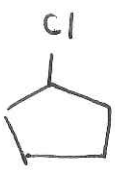
 =  cyclohexane



estrone
(female sex hormone)

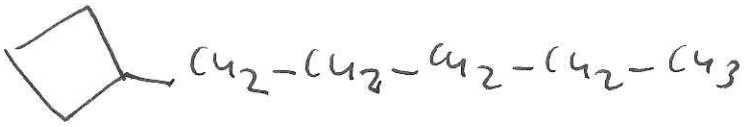
Naming

1) Find the parent by counting C atoms in the ring



chlorocyclopentane methylcyclopentane

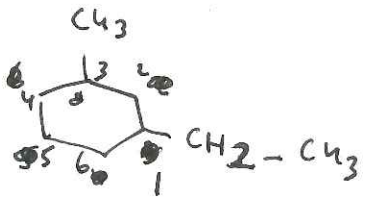
When a single ring system is attached to a single chain w a greater # of C atoms, then the compound is named as a cycloalkyl-subst. alkane, e.g.



1-cyclobutyl pentane

2-cyclopropylpentane

2) Number the substituents & write the name



1-Ethyl-3-methylcyclohexane

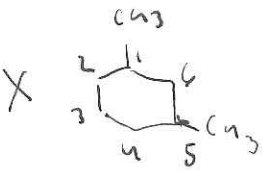
not

1-ethyl-5-methyl cyclohexane

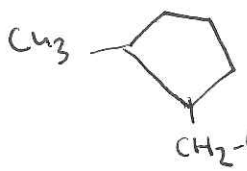
For 2 substs:

- # ring beginning with the subst first in the alphabet
- # in the direction that gives the next substituent the lower # possible

X

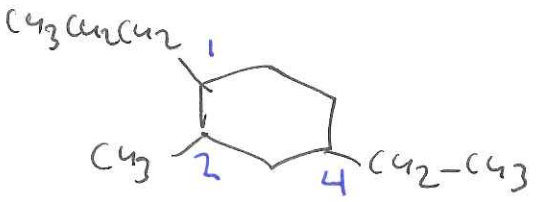


- alphabetical priority
- second subst has lower no # as possible



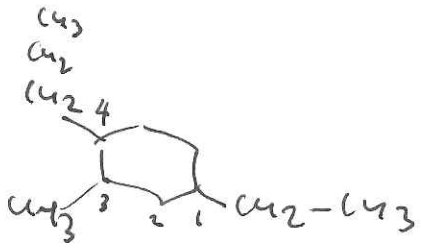
1-methyl-2-propyl cyclopentane

If there are more than 2 subst on the ring, they are cited in alphabetical order



4-ethyl-2-methyl-1-propylcyclohexane

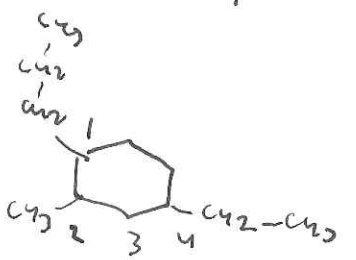
The subst. given #1 pos. is the one that results in ~~the~~ a second subst setting as low a number as possible



not 1-ethyl-3-methyl-4-propylcyclohexane

bec. 2 < 3

1,3,4

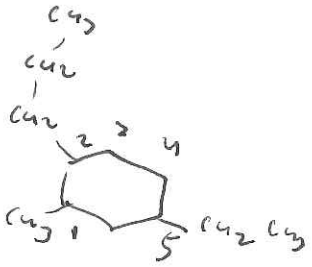


4-ethyl-2-methyl-1-propylcyclo.

*

1,2,4

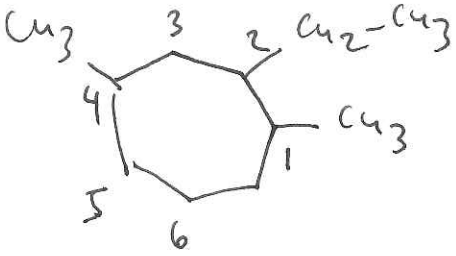
numbering was out over 1,3,4



5-ethyl-1-methyl-2-propylcyclohexane

because 4 < 5

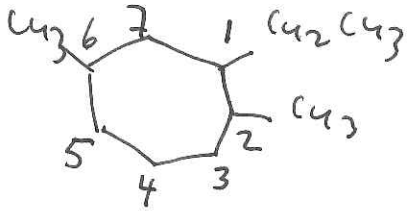
1,2,5



1,2,4

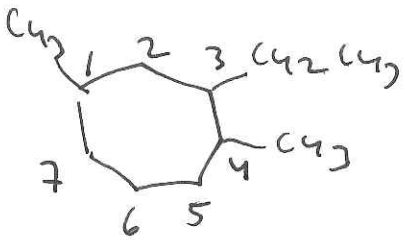
~~for 3 or more~~
~~substs, begin with~~
~~substituent~~

2-ethyl-1,4-dimethyl cycloheptane



1-ethyl-2,6-dimethyl cycloheptane

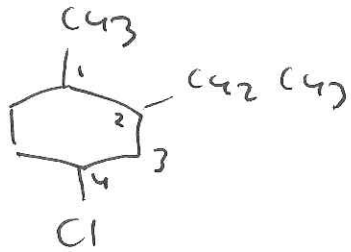
1,2,6



3-ethyl-1,4 diethyl "

1,3,4

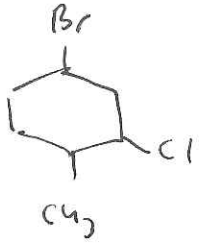
If halogens are present, treat them as alkyls:



1,2,4 numbering wins over 1,3,4 numbering 2<3

4-chloro-2-ethyl-1-methylcyclohexane

(not 1-chloro-3-ethyl-4-methylcyclohexane)



4-bromo-2-chloro-1-methylcyclohexane

Name these

Cycloalkanes: