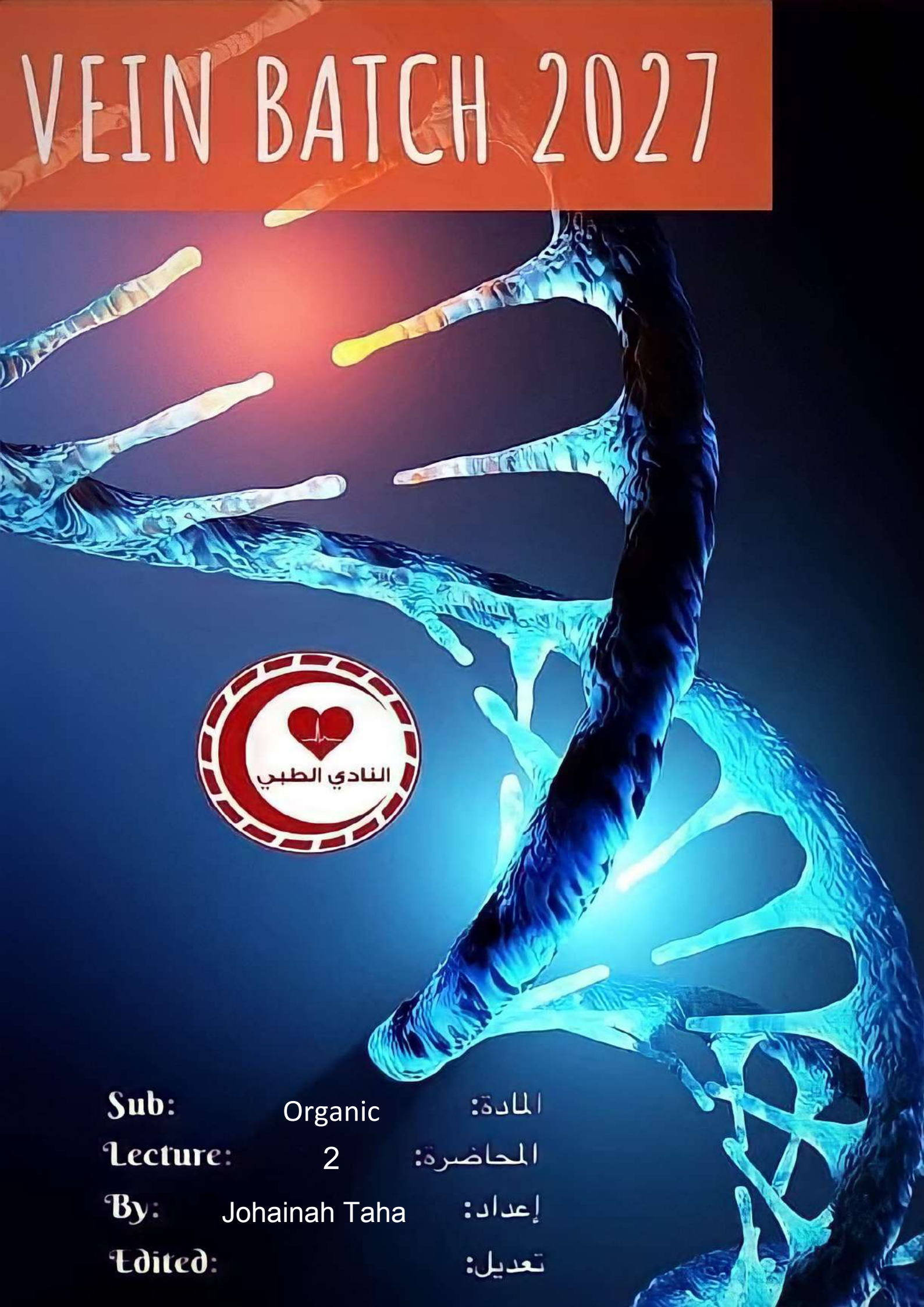
VEIN BATCH 2027



النادي الطبي

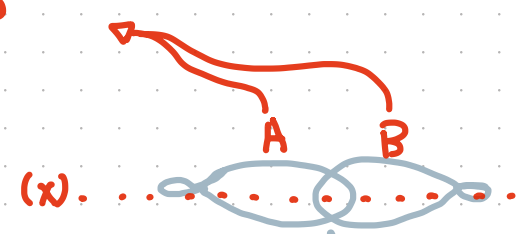
Sub:	Organic	المادة:
Lecture:	2	المحاضرة:
By:	Johainah Taha	إعداد:
Edited:		تعديل:

lecture5:

سؤال؟ شو هي ال orbitals اللي دخلناهم ببعض وعملنا هالرابطة القوية ؟

الجواب: Sp3 مع Sp3

يعني هيك شكل الرابطة



تداخل مباشر real overlaping

Segma bond

فرضاً لو حركنا B حول محور (X) بأي زاوية rotation

هل ستتأثر الرابطة Segma ؟ لا

بتسمى free rotation around segma

طيب لو عملنا rotation لطرف المركب، هل A حتضل مكانها ؟؟

لا، حيتغير مكانها، وبمعنى آخر حيظهر عندي 3D structure مختلف.

مثال:

بتسميهم rotamers أو conformers.

Conformational Isomers

shape and structure

مطابقة

Conformational isomers (rotamers or conformers) are compounds with the same constitution (atoms are bonded in the same order) but the atoms are located in different places in space.

بنية

اتفقنا انه ال rotation ما بأثر عرابطة سيغما
و لكن بكل زاوية احنا بنكون different 3 dimensional structure

ثنائي الأسطح

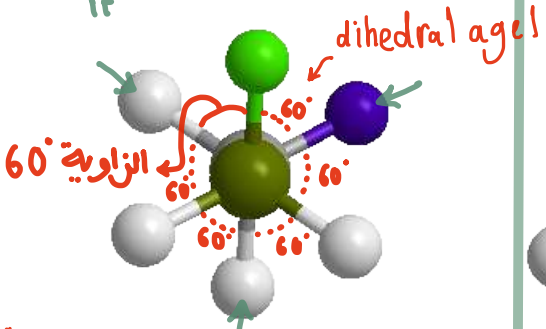
This is achieved by rotating about C-C single (s) bonds or the dihedral (or torsion) angle (q).

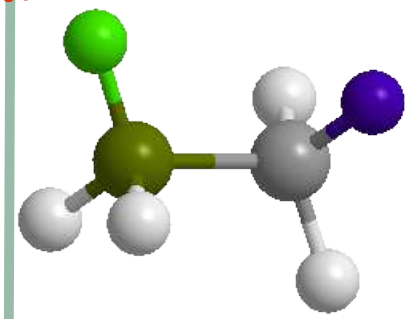
الليّ

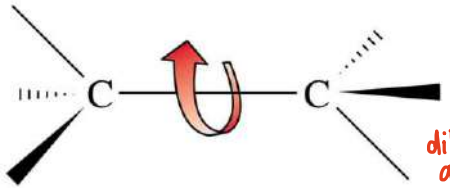
الدوران

Rotation about a **single bond** occurs easily because the amount of overlap of the *sp*3 orbitals on the two carbon atoms is unaffected by rotation about the sigma bond

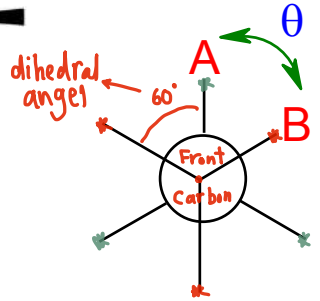
here I can't see the back carbon, but I can see the atoms around it





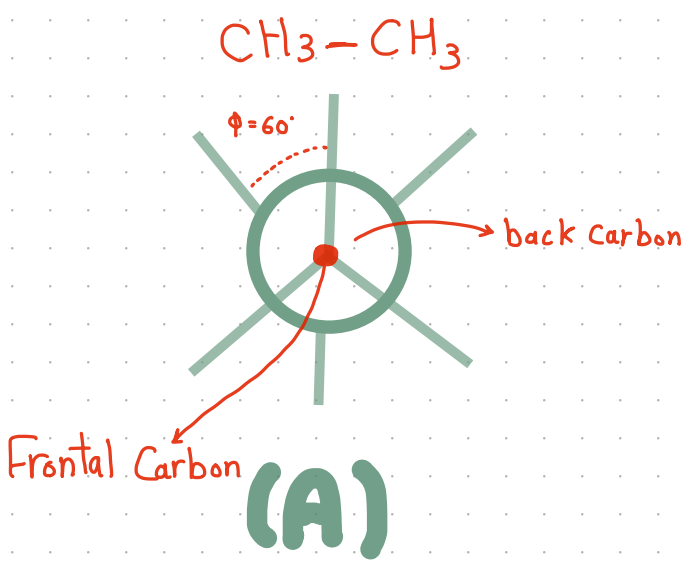


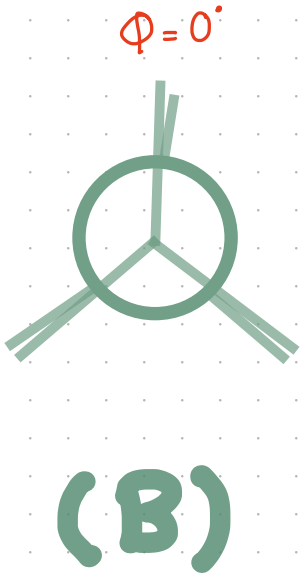
newman structure



عنا عدد لا نهائي من ال conformers ، كل ما نغير زاوية بتكون عنا new 3D structure

ولكن اهتمامنا حيكون بالرسمة A و B





- نلاحظ أن كل CH خلفه فراغ.
- Lower energy
- more stable

التفسير

Staggered

C–H

نوع الرابطة هو سيغما تكونت نتيجة تداخل مباشر بين S مع Sp^3

الذرتين تشاركوا مع بعض بإلكترون (-) بكل طرف ، طيب موسالبي وسالب تنافر؟؟ ولهذا حيصير نوع من الـ repulsions وال potension energy حتكون أعلى

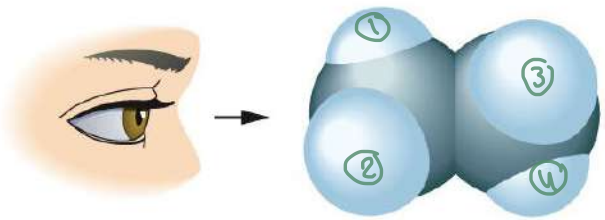
التفسير

- نلاحظ أن خلف كل CH يوجد CH
- higher energy
- less stable

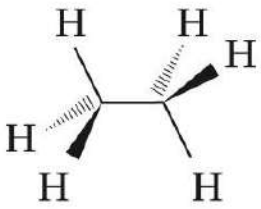
Eclipsed

Conformational Isomers (cont'd)

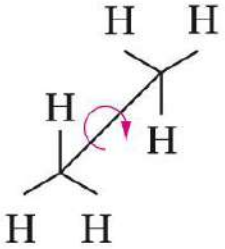
Two extremes exist for ethane: staggered & eclipsed



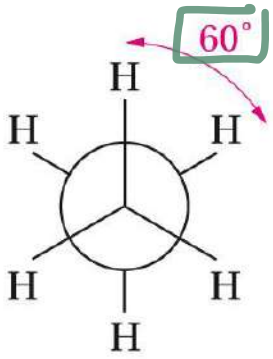
staggered



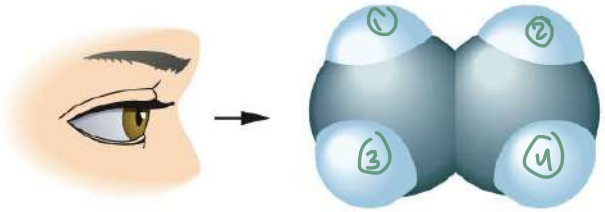
"dash-wedge"



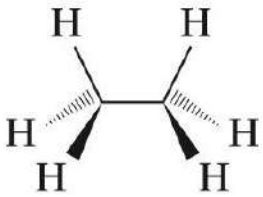
"sawhorse"



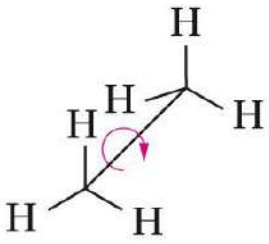
Newman



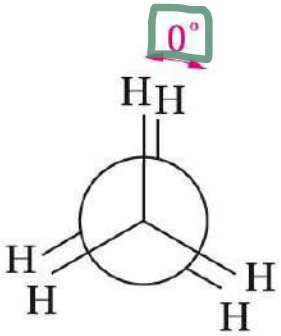
eclipsed



"dash-wedge"



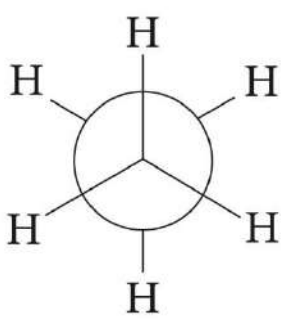
"sawhorse"



Newman

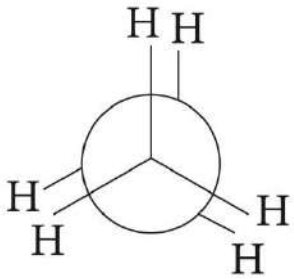
Conformational Isomers (cont'd)

These two extremes represent high and low energy "conformations" of ethane. The "high" E is the eclipsed and low E the staggered.



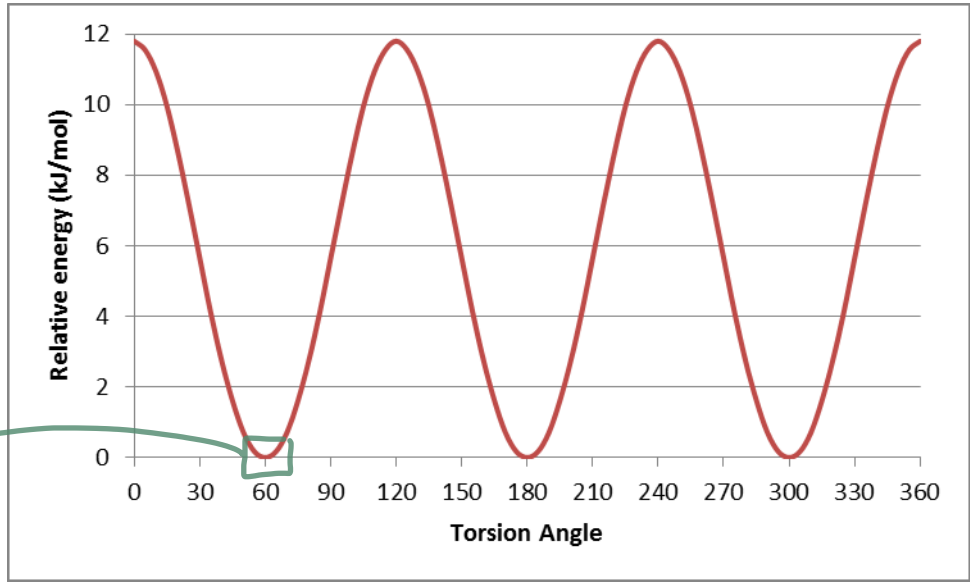
staggered

low energy



eclipsed

high energy



عند الزاوية ٦٠° بتكون أقل energy و more stable

* العلاقة بين Eclipsed و Staggered هي حالة Equilibrium *

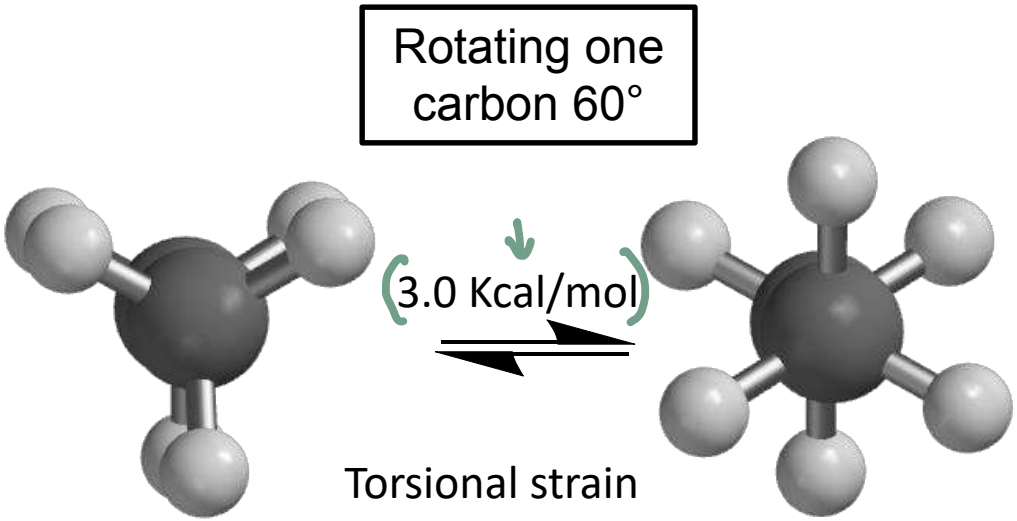
السبب يعود إلى أنه الفرق بالـ energy بينهم هو كمية كبيرة ومقدارها 3kilocalori/mole وهي كمية **قليلة** وكمان بين الـ molecules في تصادمات ممكن الـ energy تقل أو تزيد وتتحول من least stable لـ most stable والعكس.

إذاً هما في حالة اتزان

NOTE العلاقة بين energy و Stability عكسية

Conformational Isomers (cont'd)

The difference in energy is caused by "steric" interactions between the H atoms. Steric interactions are repulsions caused when two atoms are too close together in space and their valence shell electrons repel each other.



The H – H distance in the eclipsed is 2.36 Å and 2.54 Å in the staggered.

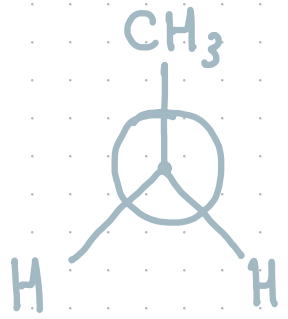
مثال $CH_3-CH_2-CH_2-CH_3$

* كما نلاحظ عنا 3 روابط سيغما
* الروابط الي بالأحمر زي بعض والي بالأخضر مختلفة.
* وأنا الآن بدي أدرس الـ Rotation الي حول الـ Segma الي بالأخضر بين:

$CH_3-CH_2-CH_2-CH_3$: Carbon 2-3

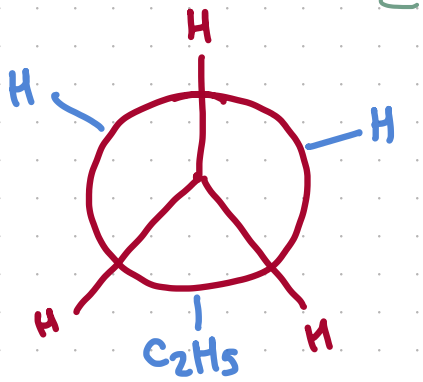
C_1 C_2 C_3 C_4

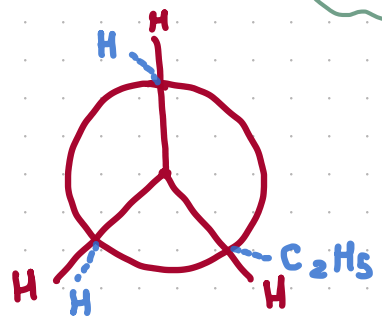
C_2 ← Front Carbon ← شابك مع ← ميثل 1 و $2H$



حلوه بعد ما تفهموا الرسم

واجبات: جرب تعمل C_1 مع C_2:

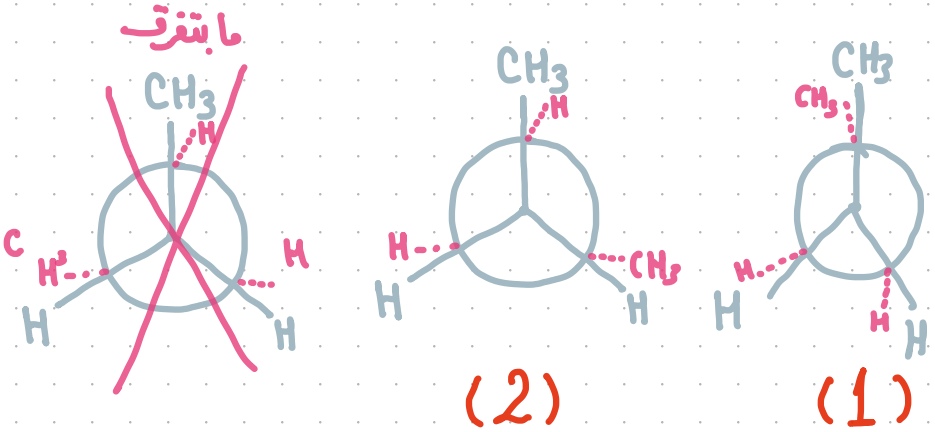




الآن، بدنا نرسم conformers للمركب: $CH_3-CH_2-CH_2-CH_3$

Front carbon

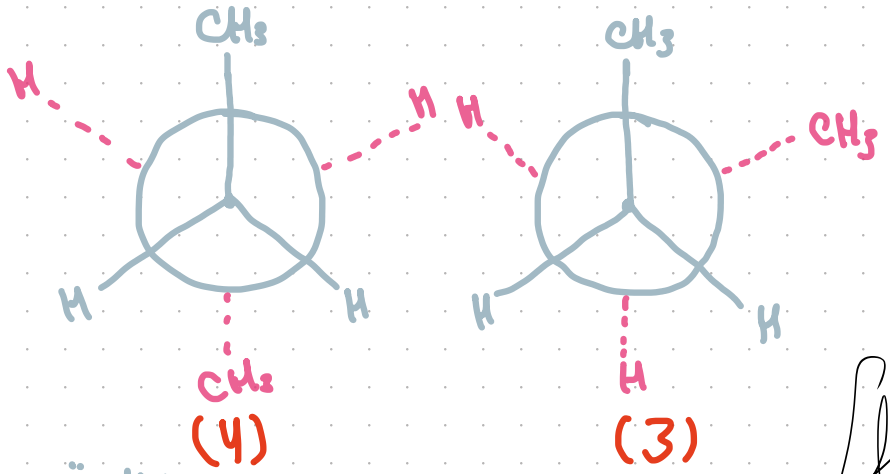
Eclipsed ①



(2) (1)

We have 2 eclipsed structures

Staggered ②



(4) (3)

2 has less energy

2 is more stable than 1

السبب ⇓

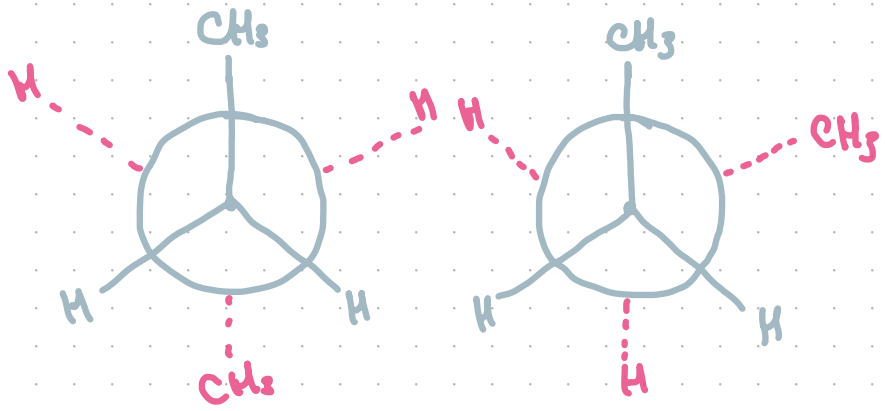
لأنو بـ 1 عم أحط مجموعة كبيرة CH_3 خلف مجموعة كبيرة (CH_3)، وهاد بنسميه Stiric factor or Stiric effect

يعني عم نعمل مضايقة و مزاحمة فراغية

4 is more stable than 3

لأنو بعدنا المجموعات الكبيرة عن بعض أكثر ما يمكن 180° و 60° و 180° = الميثل و الميثل عكس بعض الزاوية

لـ الزاوية بين CH_3 و CH_3 هي 180°



سؤال؟ بين أعلى ـــــ Stability ؟؟

4 > 3 > 2 > 1

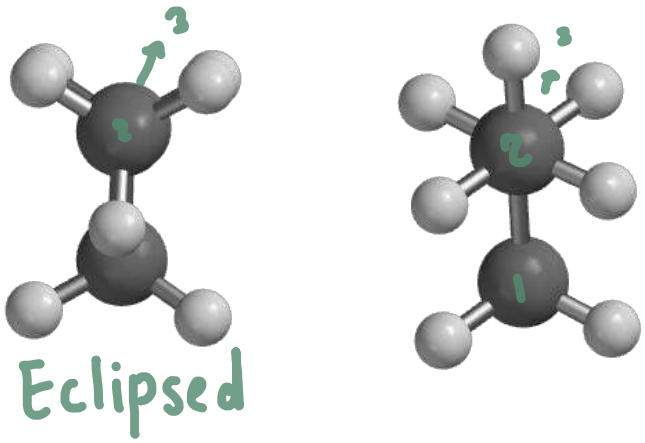
NOTE it

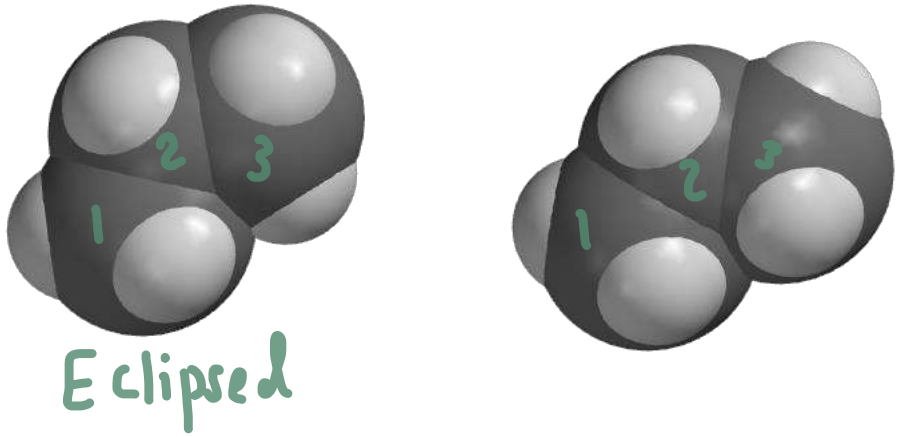
Stability عكس ال energy ال

Conformational Isomers (cont'd)

3 carbons

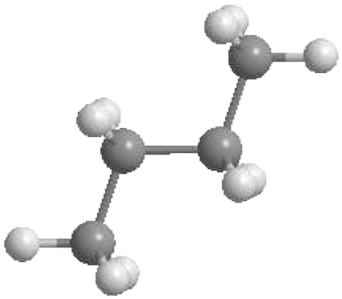
The problem is worse in propane as a methyl group is larger than a H atom. The eclipsed is on the left in both sets of images.



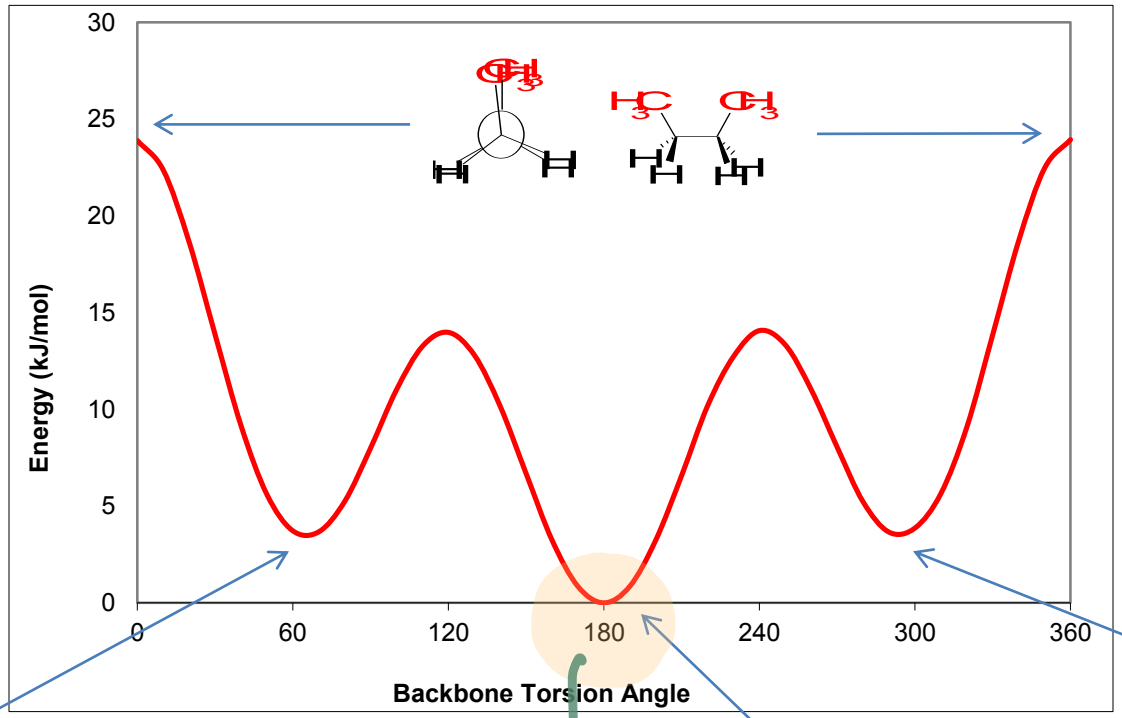


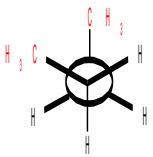
ball & stick

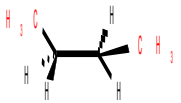
space filling



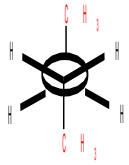
Steric effects reach their maximum in butane:

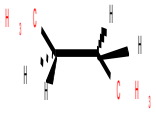


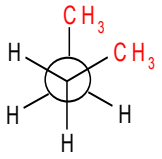


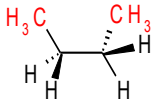


More Stable مثل ماشرحنا









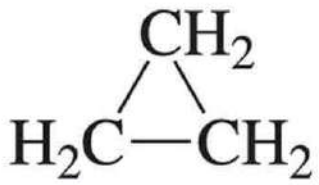
2.9 Cycloalkane Nomenclature and Conformation

Cycloalkanes are saturated hydrocarbons that have at least one ring of carbon atoms. The general formula is C_nH_{2n}.

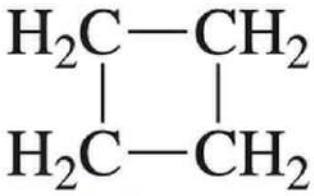
Single bond

without +2

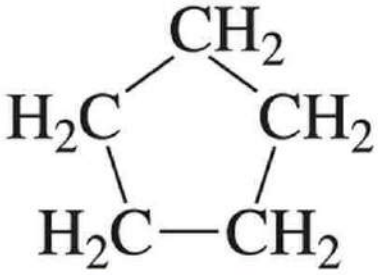
Note we don't have cyclo ← methan. / Ethan.



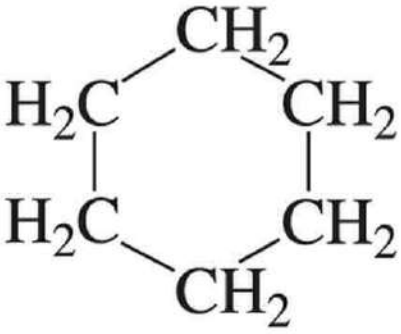
cyclopropane



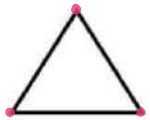
cyclobutane



cyclopentane



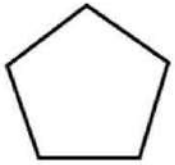
cyclohexane



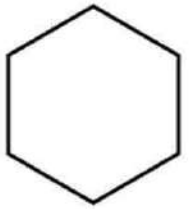
cyclopropane

CH_2 كل نقطة *

cyclobutane



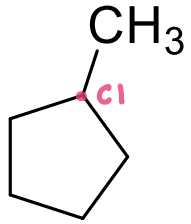
cyclopentane



cyclohexane

Cycloalkane Nomenclature

- **One substituent** is always located at ring carbon number 1. A number is not needed.



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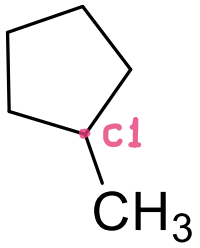
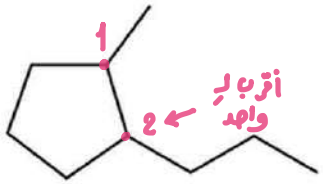


methylcyclopentane

methylcyclopentane

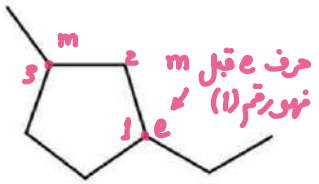
لايكون عنا تفرع واحد ماني
داعي للأرقام ، أما التفرعين
لازم أرقام

Two substituents : Substituents are stated in alphabetical order. #1 goes to the first-listed substituent

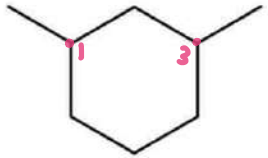


1-methyl-2-propylcyclopentane

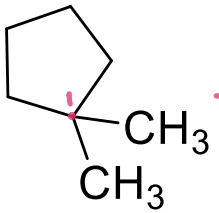
m قبل p فبالتالي
هي رقم واحد ت



1-ethyl-3-methylcyclopentane



1,3-dimethylcyclohexane



→ 1,1-dimethylcyclopentane

الآن بدنا نقارن بين cycloalkene و normal alkane من ناحية energy, conformers, stability:

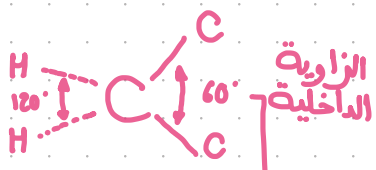
(الوضع الـ normal)

- more stable → tetrahydral structure
- less repulsion → التفاعل بين الأذلاك أضعف مايمكن
- Θ = 109.5°

sp3 s

Good overlapping → strength bond

لو قللنا الزاوية عن 109.5 ، اعتماد من السلايد والقادم:



بعيدة عن ideal angle = 109.5° ← يسبب ← poor overlapping ← weak bond

angle strain ← تسبب مايسمى

deviation ← جهد حدث بسبب ← ideal angel

مثلاً 60° بعيد كثير عن 109°

فبالتالي الـ angle strain تبعه عالي

الملخص 😁😁

ال ideal angle = 109

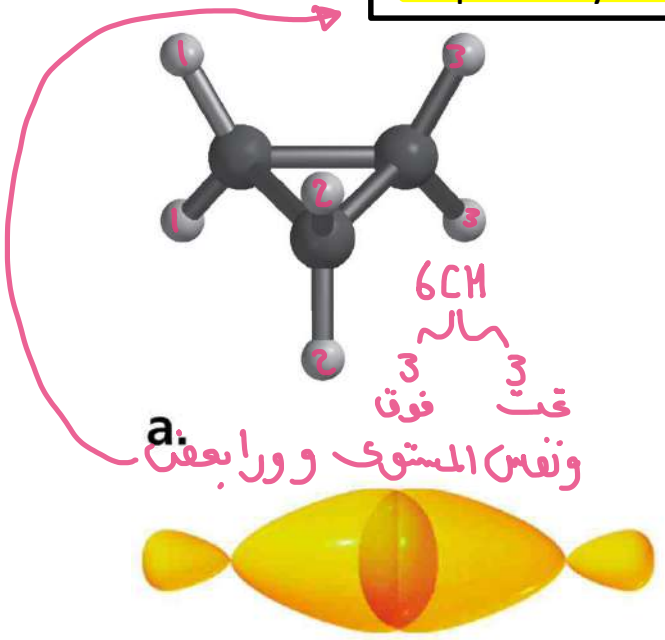
و هي الزاوية الي بكون عندها المركب فيه good overlapping فبالتالي strong bond

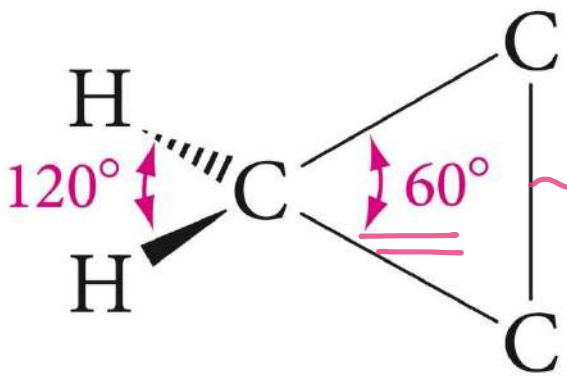
لو تغيرت الزاوية و بعدت عن ideal angle يؤدي ذلك الى poor overlapping فبالتالي weak bond

Cycloalkanes: cyclopropane – is the smallest ring structure possible.

- It is rigid and very highly **strained** as the bond angles (60°) are distorted from ideals (109.5°)
- It is more reactive than a linear alkane as the strained C-C bonds are easier to break

Eclipsed Hydrogens





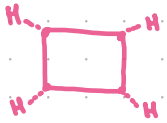
torsional strain بنسميها
الطاقة الي بتكلفني لأنتقل من
more stable(staggered) لِ
less stable (eclipsed)

Angle strain + Torsional strain = Ring strain

Angle strain results from poor orbital–orbital overlap because bonds have to deviate from the ideal (109.5°) bond angle

Cyclobutane :

* حلقة رباعية.
* الزاوية فيه بتكون 90° ، نعم هي بعيدة عن 109° ولكن ليست بسوء الـ 60°
* من عند cyclobutane واللي بعدها ببلش الـ molecules يعمل conformers معينة ، بحيث إنه يعمل twisting و لحتى مايضل بنفس الـ planer بيحاول يشيل نفسه بطريقة معينة. حيث يعطي نفسه شكل معين ، والفكرة منيط انو نعمل minimize لـ eclipsing ؛ لانو كل CH مقابلة CH لما نحرك الكربونة أحنا بنعمل orientation لـ CH فبيطلوا مقابلين لبعض



فأنا لما أعمل twisting بـ cyclobutan انا عم أخفف من eclipsing ولكن ما بتختفي منهم.

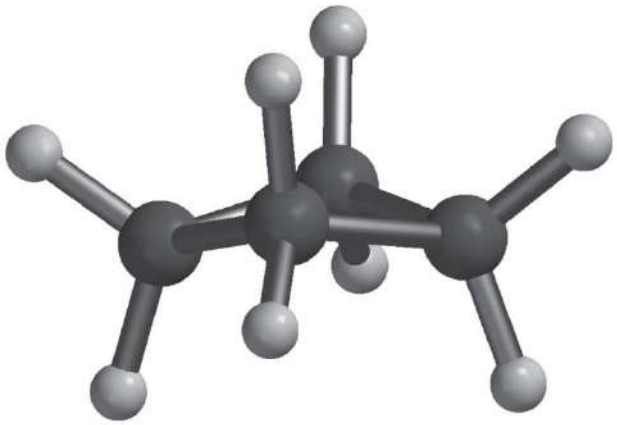
باختصار، أنا بغير اتجاه H حتى التالي بقلل من Eclipsing وبقلل كمان من Angle strain

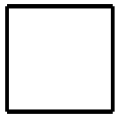
Cyclobutane

Cycloalkanes: cyclobutane – "puckered" conformation

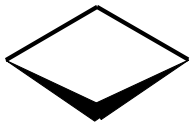
- It is more flexible than cyclopropane and is not flat although it is commonly drawn that way.
- It is more reactive than a linear alkane as the strained C-C bonds are easier to break, bond angle ~90°

* Stability in cyclobutan > cyclopropane
* Angle strain + torsional strain





common



better

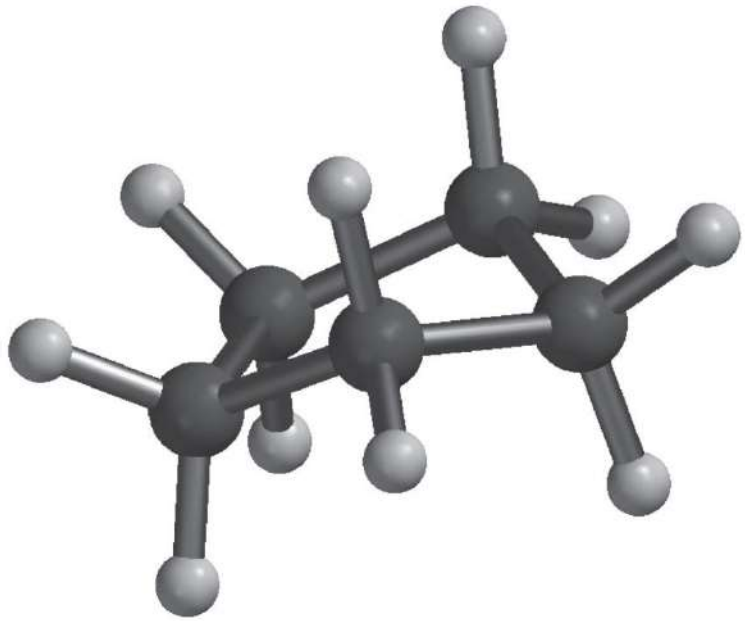
Molecules twist out of a planar arrangement to ① minimize angle strain and ② the number of eclipsed hydrogens

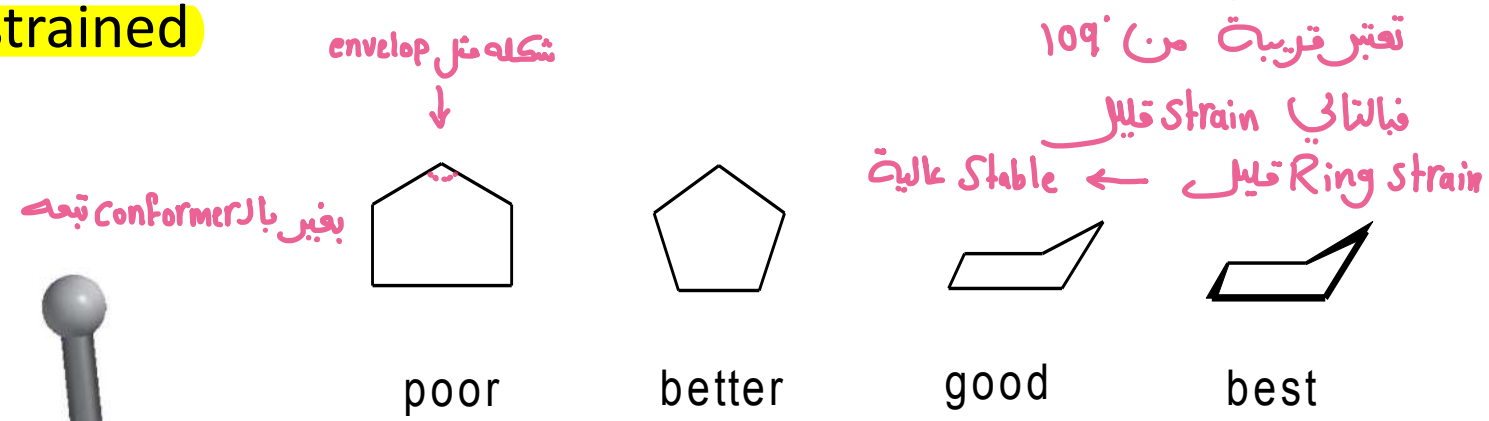
هنا اقل من cyclopropane

cyclopentane

Cycloalkanes: cyclopentane – "envelope" conformation

- It is more flexible than cyclobutane and bond angle are ~105°, and less strained





Molecules twist out of a planar Arrangement to minimize angle strain and the number of eclipsed hydrogens.

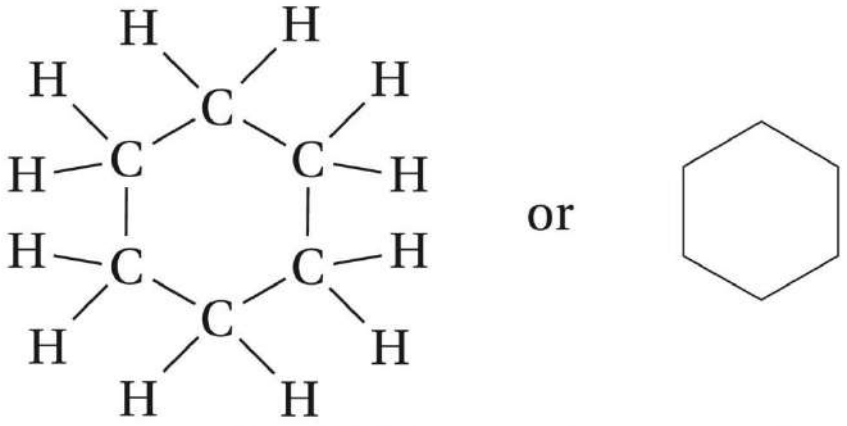
cyclohexane

Cycloalkanes: cyclohexane – "chair"

- It is highly flexible and can adopt a **strain free** non-planar conformation with bond angle of 109.5°
- It is very common in nature so understanding its conformations is important.

Chair يتخذ conformer هيكل بنسبية

Although commonly drawn as a hexagon, implying a flat six-membered ring this is not the common conformation seen.



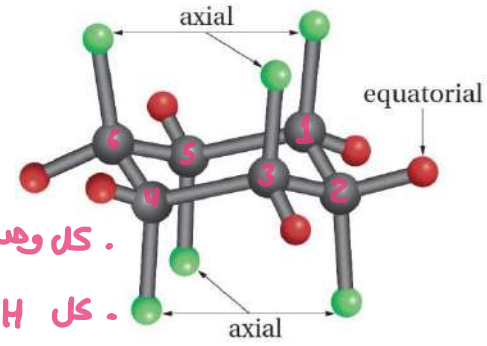
Structural and abbreviated structural formulas for cyclohexane

Conformational Isomers (cont'd)

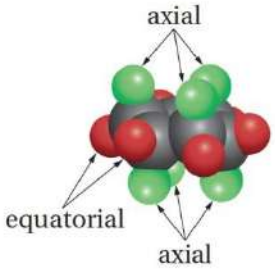
Cyclohexane cont'd:

The most common conformation of cyclohexane is the "chair" conformation. In this geometry the C bonds are all ~109.5° as opposed to the 120° in a planar structure.

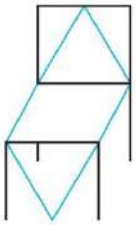
الزاوية بين C



ball-and-stick model



space-filling model


(chair framework)
(has a chair shape)

- no angle strain.
- all CH are staggered.
- no torsional strain.
- Ring strain → Free = Zero
- no Eclipsing Carbons.
- The most stable cycloalkan.

كل وحدة بمستوى مختلف.

كل CH ← staggered.

This structure creates two subsets of hydrogen atoms, those lying in the same plane as the C atoms, the equatorial H and those lying above and below that plane, the axial H atoms

Cycloalkan → Saturated
→ C_nH_{2n}

-: cycloalkan ملخص بسيط على *

* Ideal angle = 109.5°

	Cyclopropane	cyclobutane	cyclo bentane	cyclo hexan
Strain angle	60°	90°	105°	109.5°
more strain	>	>	>	X
Eclipsed Hydroge	>	>	>	X
torosional strain	✓	✓	✓	X
Flexibility	<	<	<	
Stability	<	<	<	
Energy	>	>	>	
Staggered	X	<	<	<
Shape	The smallest cycloalkan	puckered	Envelop	Chair

New vocabulary 🥰

- constitution: بنية
- repel: ابعاد
- stability: استقرار
- rotation: دوران
- dihedral angle = torsion angel
- staggered: لما الذرات ما تكون عنفس المستوى
- eclipsed: لما الذرات تكون عنفس المستوى
- repulsion: تنافر
- overlapping: تداخل
- distorted: انحراف

لا تتسلق الجبال ليراك العالم
تسلقها لكي ترى أنت العالم

بالتوفيق...
زميلتكم: جوينة لمه