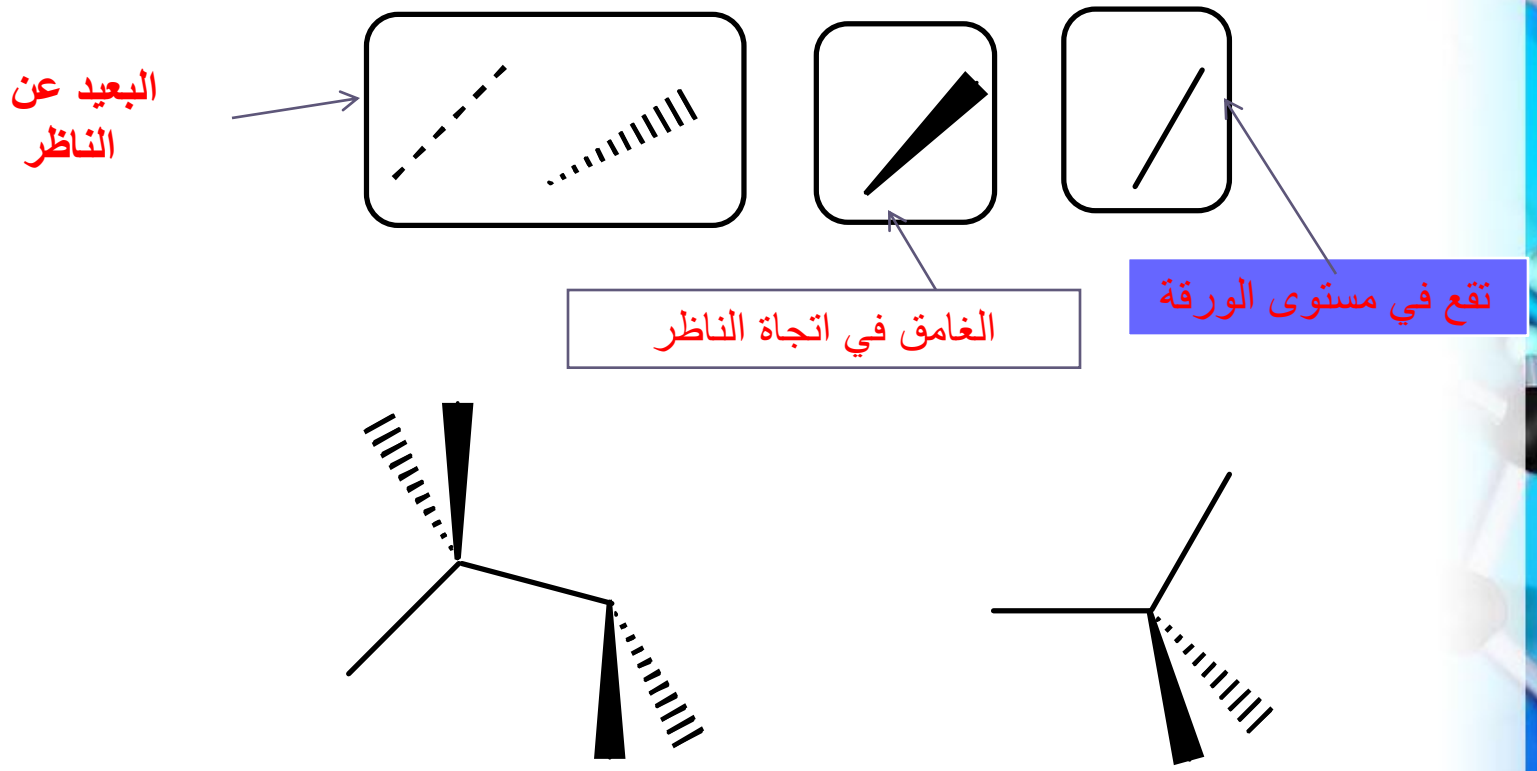
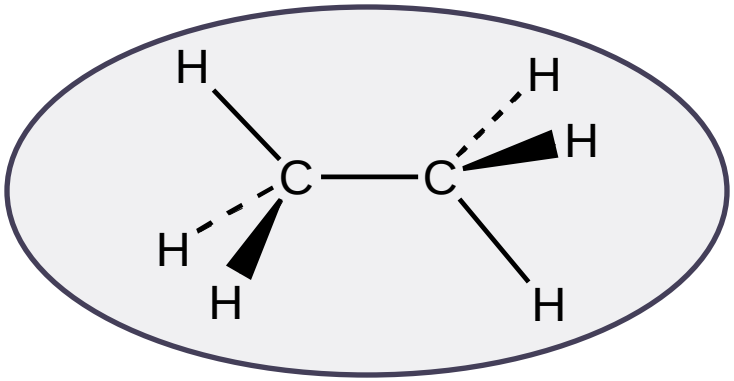
الفصل السادس :

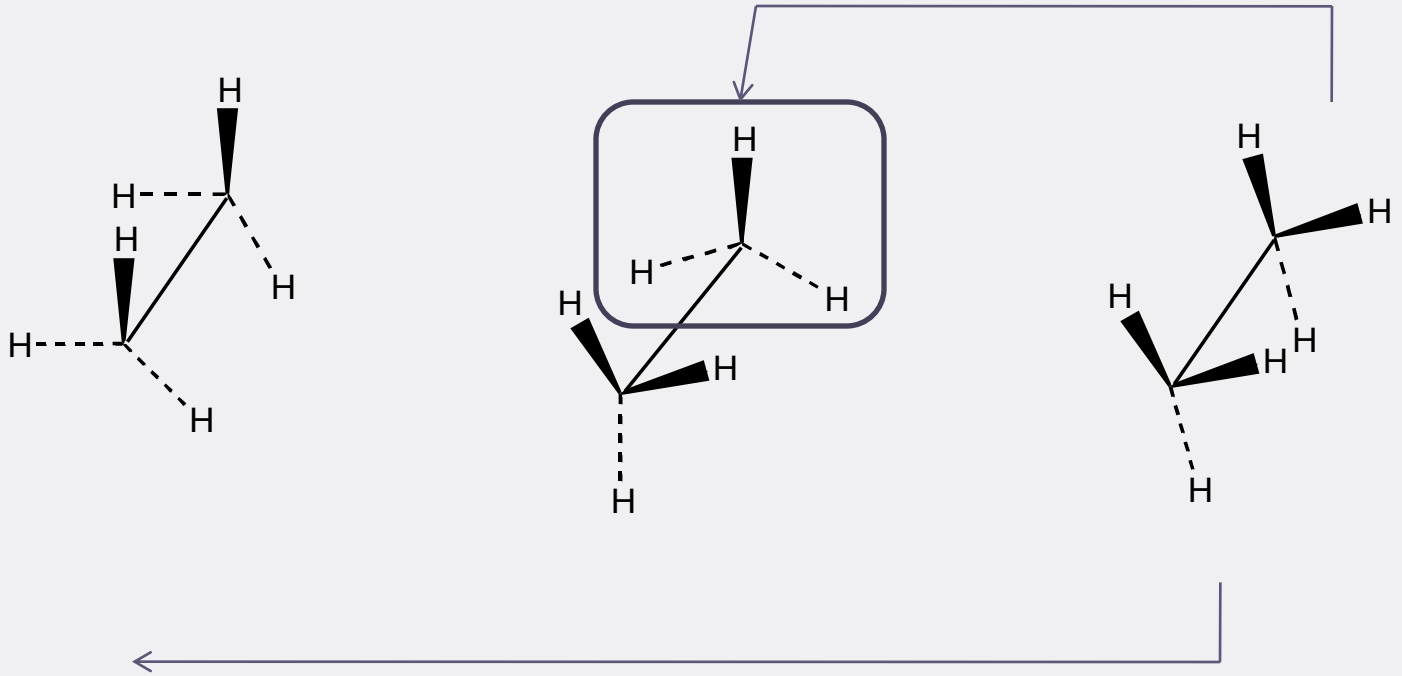
تمثيل الجزيئات العضوية فراغياً على الورق

Perspective الرسم المنظوري

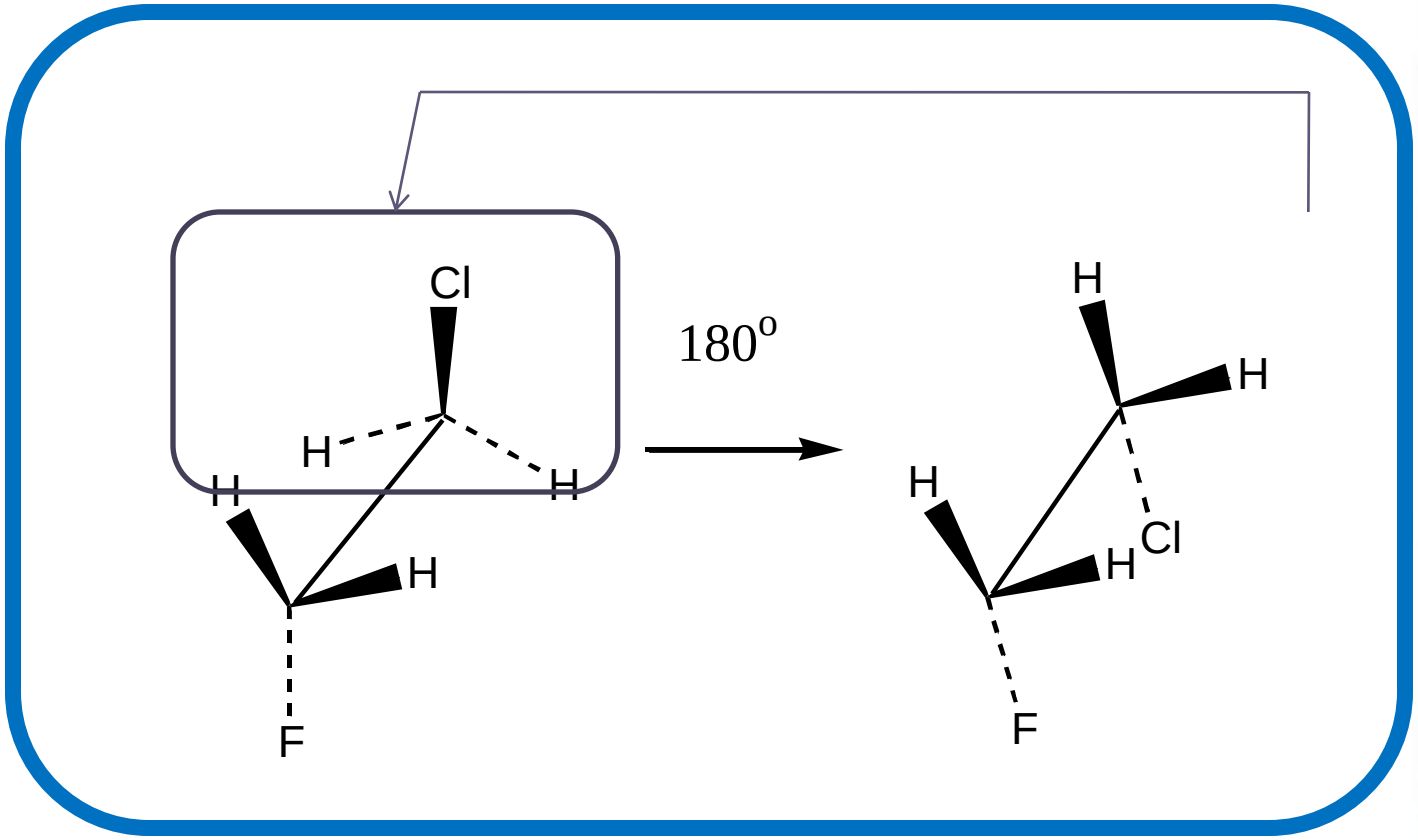




دوران حول ذرة كربون واحدة



دوران للجزئ كامل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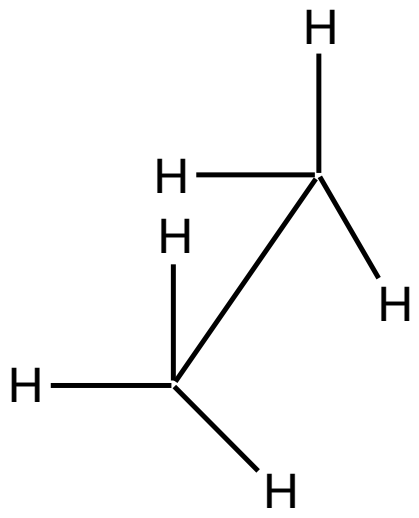
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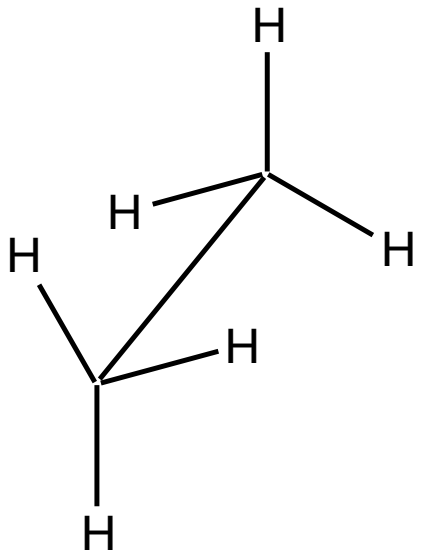
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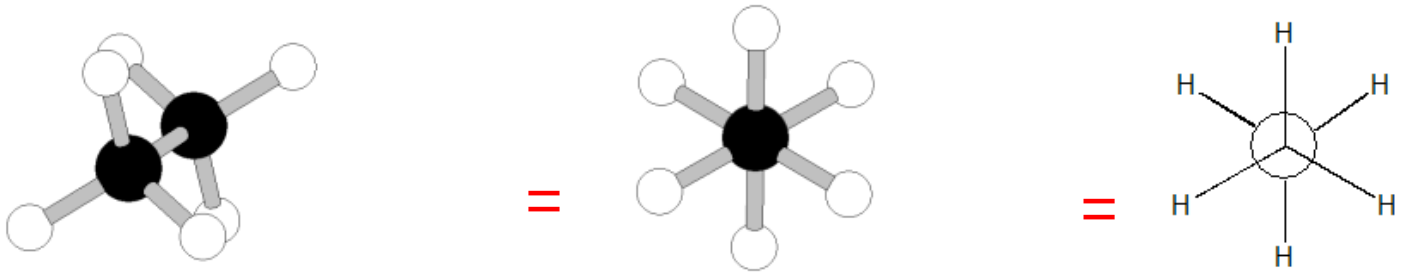
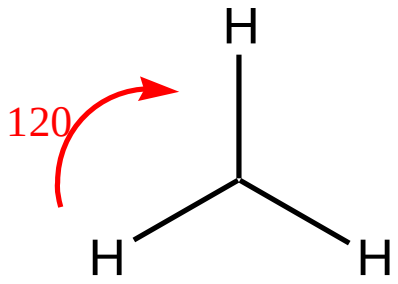
مسقط نيومان
Newmann Projections



Newmann projection

مسقط نيومان
Newmann Projections

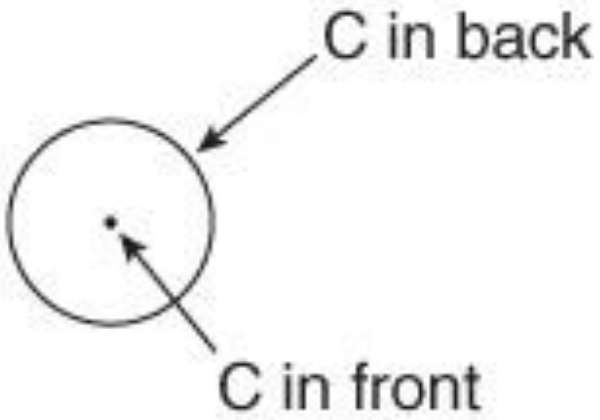
- لعمل مسقط نيومان لجزء الإيثان CH_3CH_3
- **نتبع الخطوات التالية : الخطوة الأولى :**



- End-on representations for conformations are commonly drawn using a convention called a Newman projection.

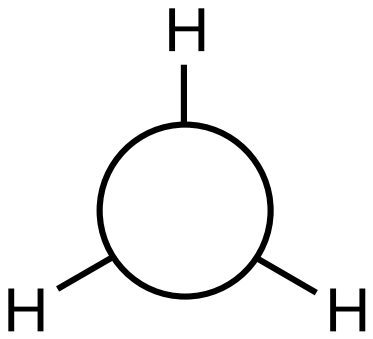
Step 1. Look directly down the C—C bond (end-on), and draw a circle with a dot in the center to represent the carbons of the C—C bond.

=



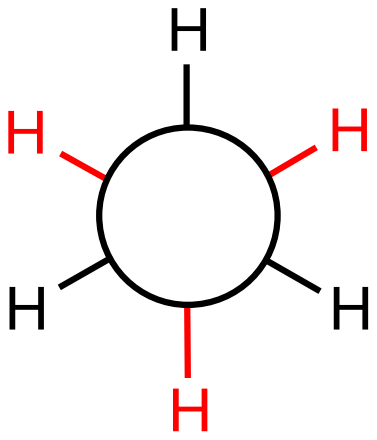
Newmann Projections مسقط نيومان

2- الخطوة الثانية



Newmann Projections مسقط نيومان

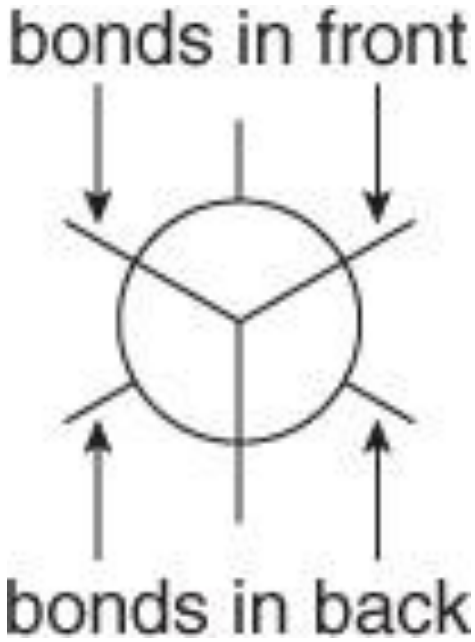
- 3- الخطوة الثالثة :

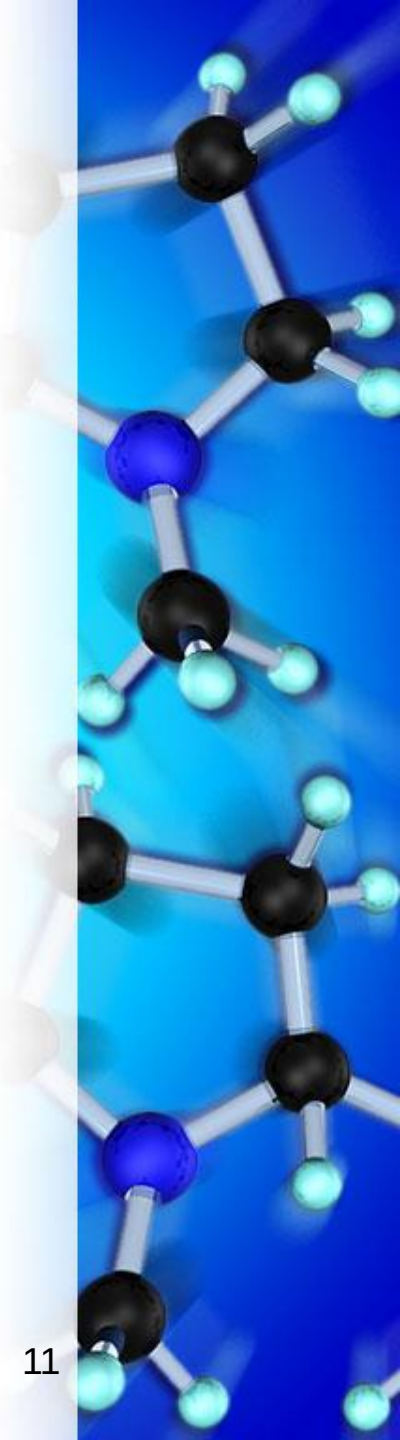


Step 2. Draw in the bonds.

Draw the bonds on the front C as three lines meeting at the center of the circle.

Draw the bonds on the back C as three lines coming out of the edge of the circle





Step 3. Add the atoms on each bond.

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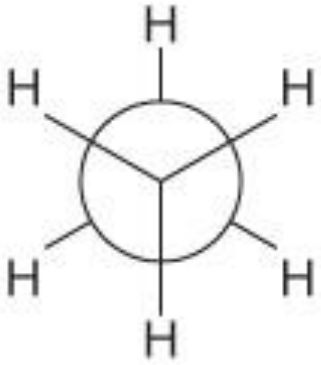
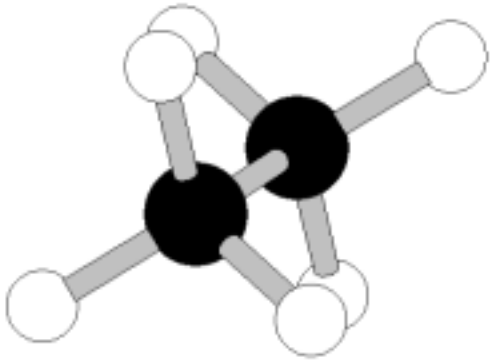
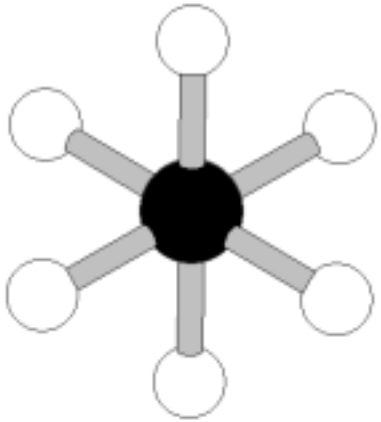
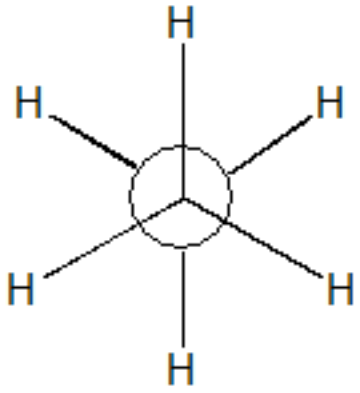


Each C has 3 H's in ethane.

Newmann Projections



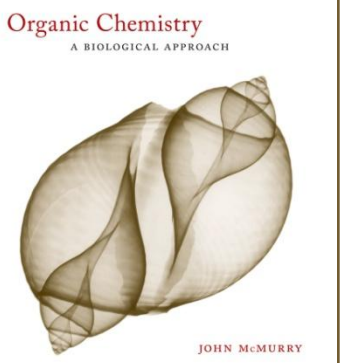




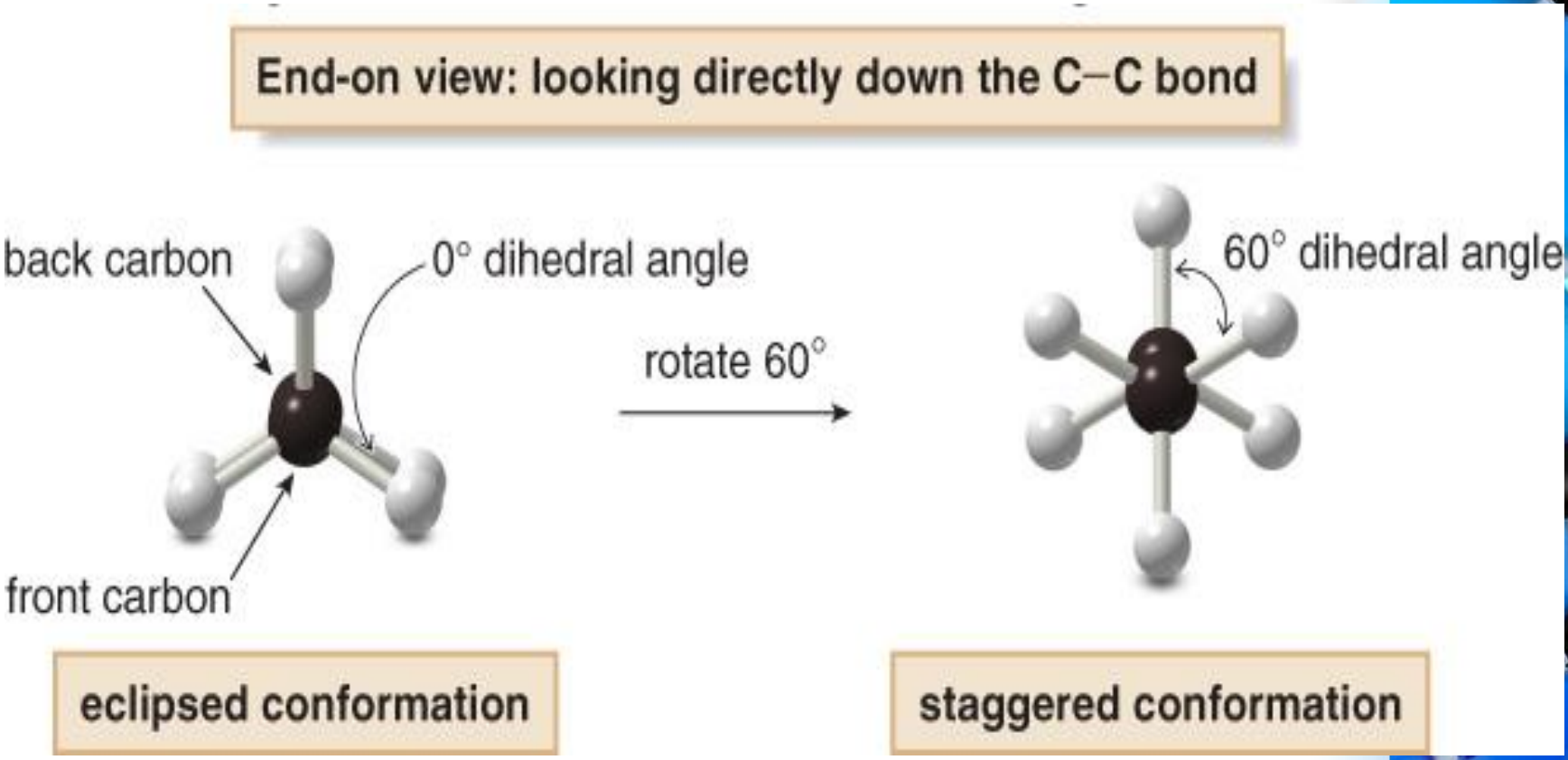
Newmann projection

تحليل الهيئة للمركبات المفتوحة
Conformation isomers

الترتيب الذري للذرات كافة او المجموعات الذرية و الترتيب هذا يتوقف على دوران ذرة الكربون حول الرابطة الأحادية



- Rotating the atoms on one carbon by 60° converts an eclipsed conformation into a staggered conformation, and vice versa.
- The angle that separates a bond on one atom from a bond on an adjacent atom is called a dihedral angle. For ethane in the staggered conformation, the dihedral angle for the C—H bonds is 60°. For eclipsed ethane, it is 0°.



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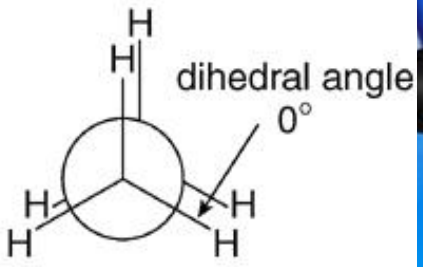
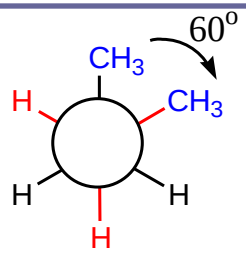
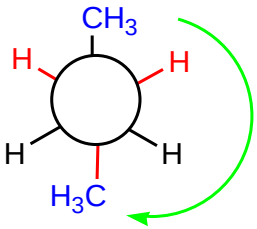


eclipsed conformation





Anti

Staggered conformation

Skew conformation الأفلاك المائلة

تشكيل الهيئة لجزي الايثان

Conformations of Ethane

Conformations of Ethane تشكيل الهيئة لجزي الايثان

Stability of conformations

- Perfectly free rotation is not observed in ethane
- Some conformations are more stable than others

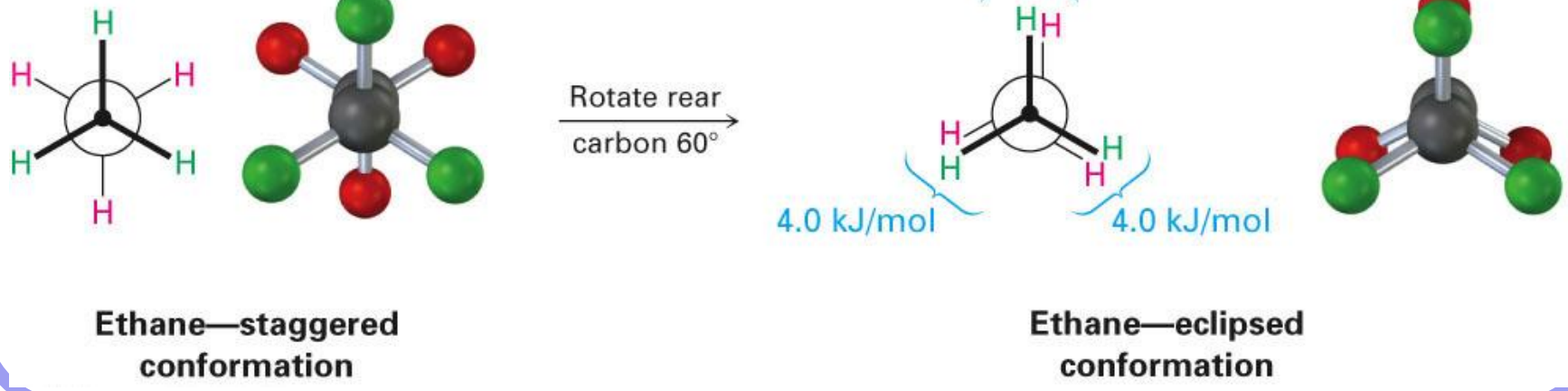
Newman projections

Staggered

- Lowest energy, most stable conformation
- All six C-H bonds are as far away from one another as possible

Eclipsed

- Highest energy, least stable conformation
- The six C-H bonds are as close to one another as possible



تشكيل الهيئة لجزي الايثان

Conformations of Ethane

منحنى الطاقة

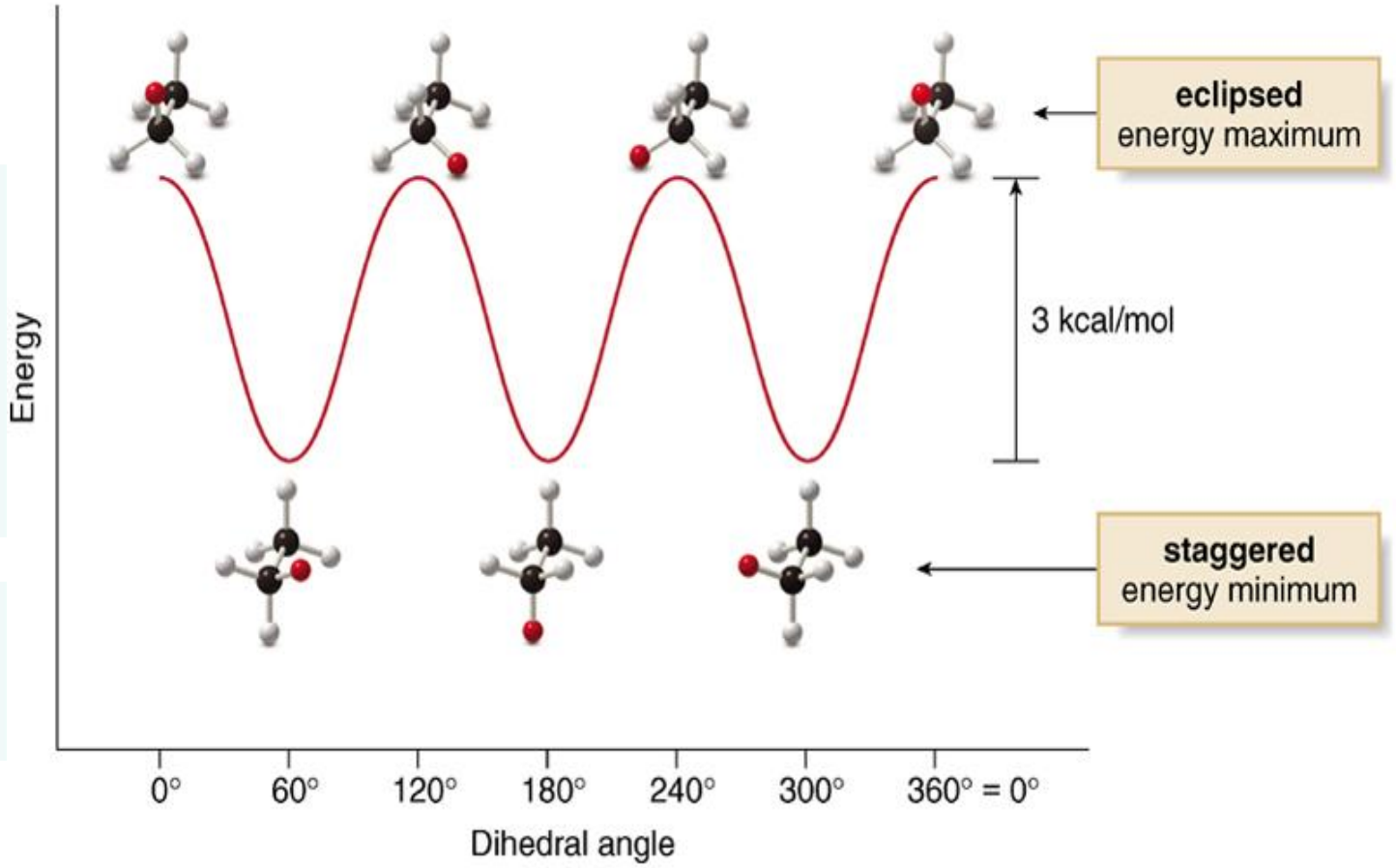
نتيجة دوران إحدى ذرات الكربون حول الرابطة سيجما بينهما بزاوية ما يتبين أن الوضع الكسوفي eclipsed أعلى بالطاقة الكامنة و أن الوضع التعاقبيstaggered نتيجة الدوران **60** أو **180** درجة اقل بالطاقة الكامنة و يرجع ذلك للتوتر **strain** و سميت الطاقة بطاقة التوتر **strain energy** أو طاقة توتر الفتل أو الدوران **torsional strain energy**

- The difference in energy between staggered and eclipsed conformers is ~3 kcal/mol, with each eclipsed C—H bond contributing 1 kcal/mol. The energy difference between staggered and eclipsed conformers is called torsional energy.
- Torsional strain is an increase in energy caused by eclipsing interactions.

Figure: Graph: Energy versus dihedral angle for ethane

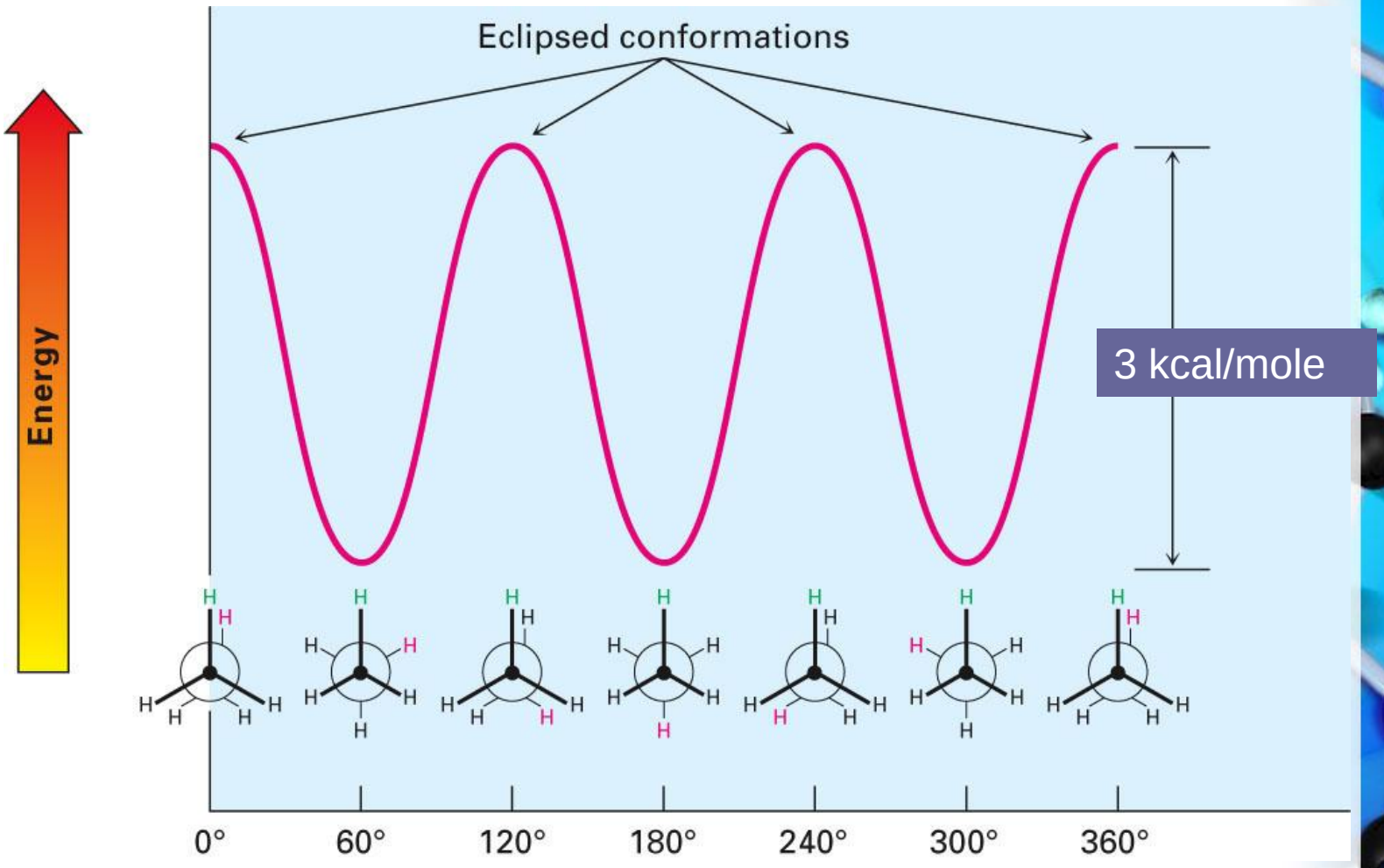
At any given moment, all ethane molecules do not exist in the more stable staggered conformation; rather, a higher percentage of molecules is present in the more stable staggered conformation than any other possible arrangement.

Each H,H eclipsing interaction contributes 1 kcal/mol of destabilization to the eclipsed conformation.



- Note the position of the labeled H atom after each 60° rotation. All three staggered conformations are identical (except for the position of the label), and the same is true for all three eclipsed conformations.

- Energy **minima** occur at **staggered** conformations
- **Energy maxima** occur at **eclipsed** conformations



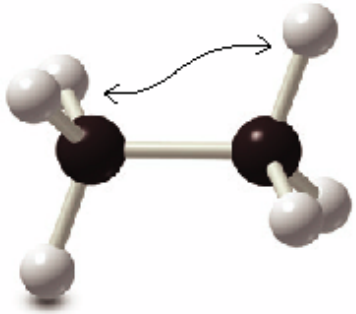
- The staggered and eclipsed conformations of ethane interconvert at room temperature, but each conformer is not equally stable.
- The staggered conformations are more stable (lower in energy) than the eclipsed conformations.
- Electron-electron repulsion between bonds in the eclipsed conformation increases its energy compared with the

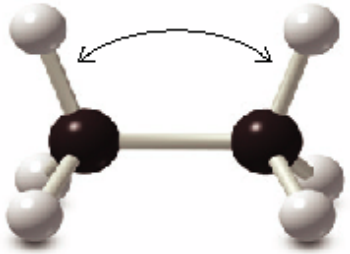
بعيدة عن بعضها البعض C-Hالروابط

قريبة عن بعضها البعض C-Hالروابط

These C—H bonds are farther apart.

These C—H bonds are closer together.





staggered conformation
side view

eclipsed conformation
side view

more stable

less stable

اكثر ثباتاً

اقل ثباتاً

تشكيل الهيئة للإلكانات المفتوحة

(غير الحلقية)

Conformations of Acyclic Alkanes

تشكيل الهيئة لجزي البروبان

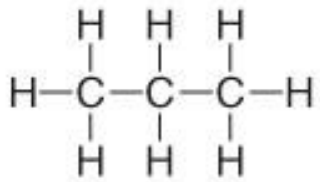
Conformations of Butane

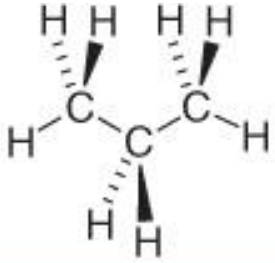
تشكيل الهيئة لجزي البروبان
Conformations of Butane

- The three-carbon alkane $CH_3CH_2CH_3$, called propane, has a molecular formula C_3H_8. Note in the 3-D drawing that each C atom has two bonds in the plane (solid lines), one bond in front (on a wedge) and one bond behind the plane (on a dashed line).

$CH_3CH_2CH_3$
propane

=





Lewis structure

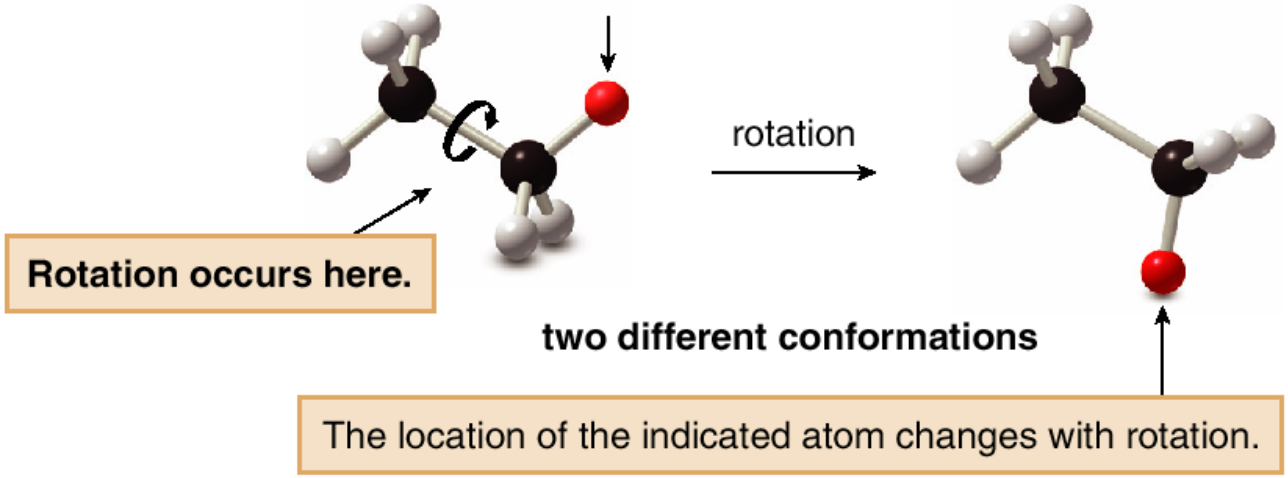
3-D representation

ball-and-stick model

Conformations of Butane تشكيل الهيئة لجزي البروبان

- Imagine looking down the bond between the two central atoms of butane (the C2-C3 bond). Use Newmann projections to draw the four conformers:

  You will calculate the energies of these four conformers in lab. For now, rank them from lowest energy (most stable) to highest energy (least stable).

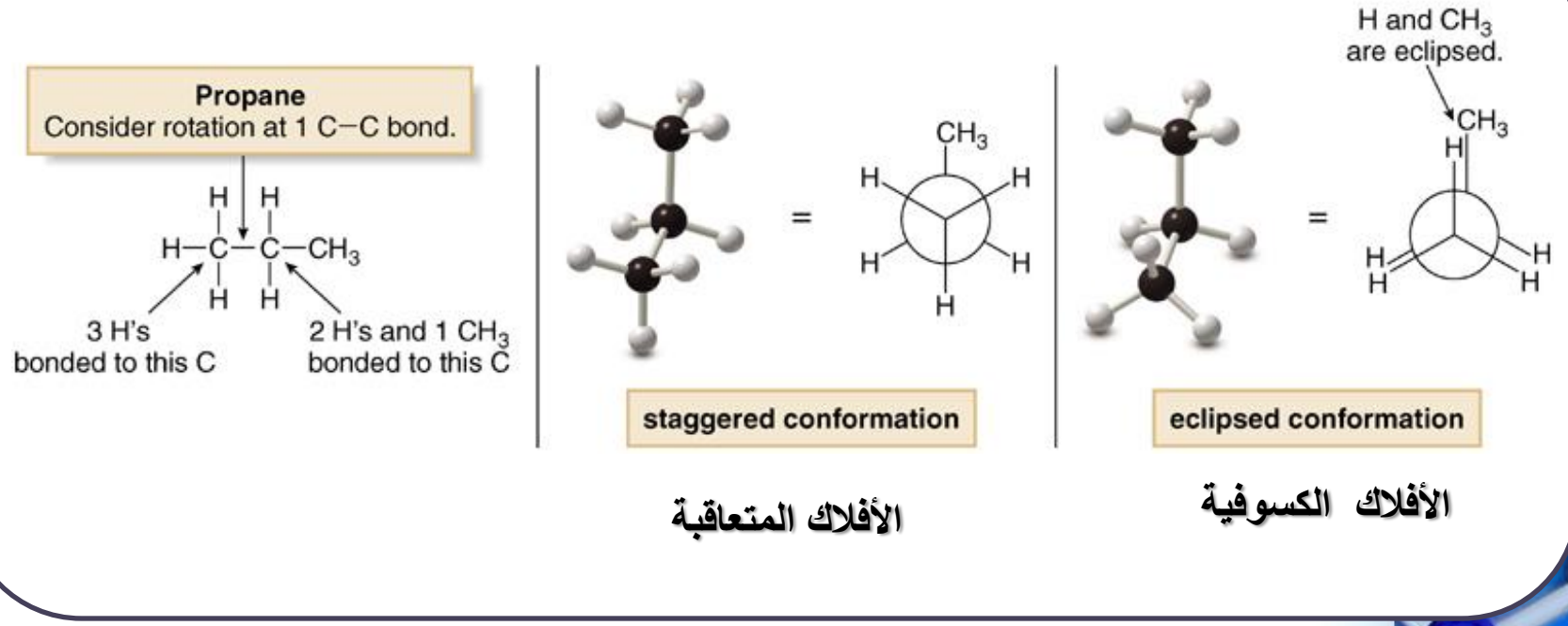


- *Conformations* are different arrangements of atoms that are interconverted by rotation about single bonds.

Conformations of Butane تشكيل الهيئة لجزي البروبان

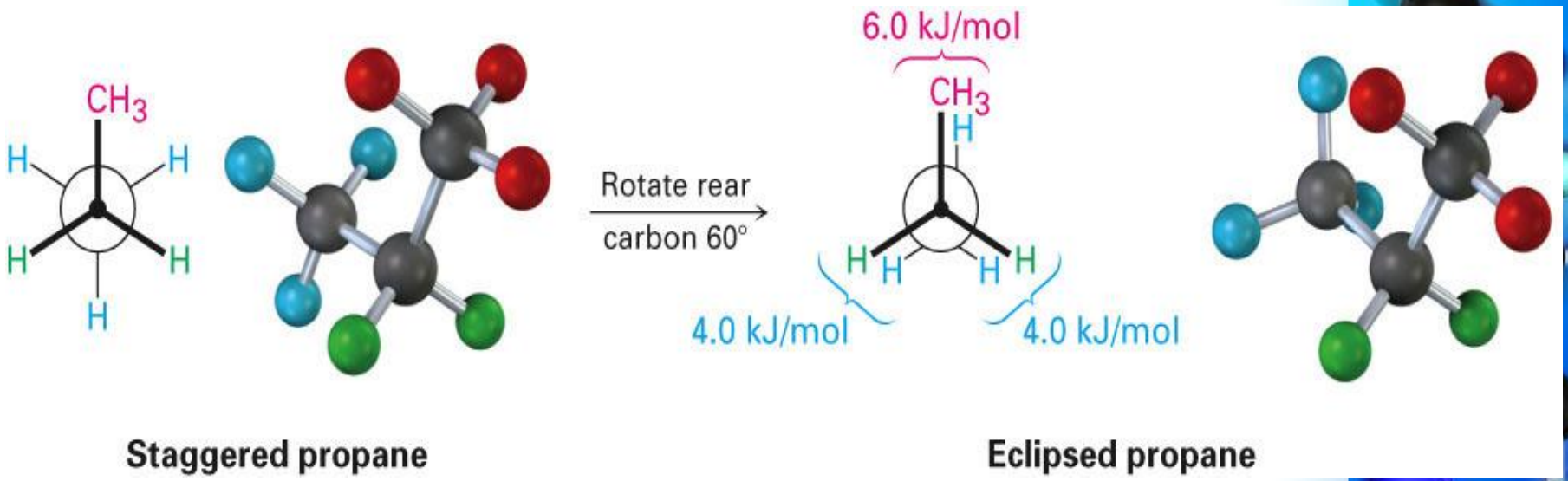
تمثيل جزئ البروبان بواسطة نيومان توضح الافلاك الكسوفية و المتعاقبة في البروبان

Newman projections for the staggered and eclipsed conformations of propane

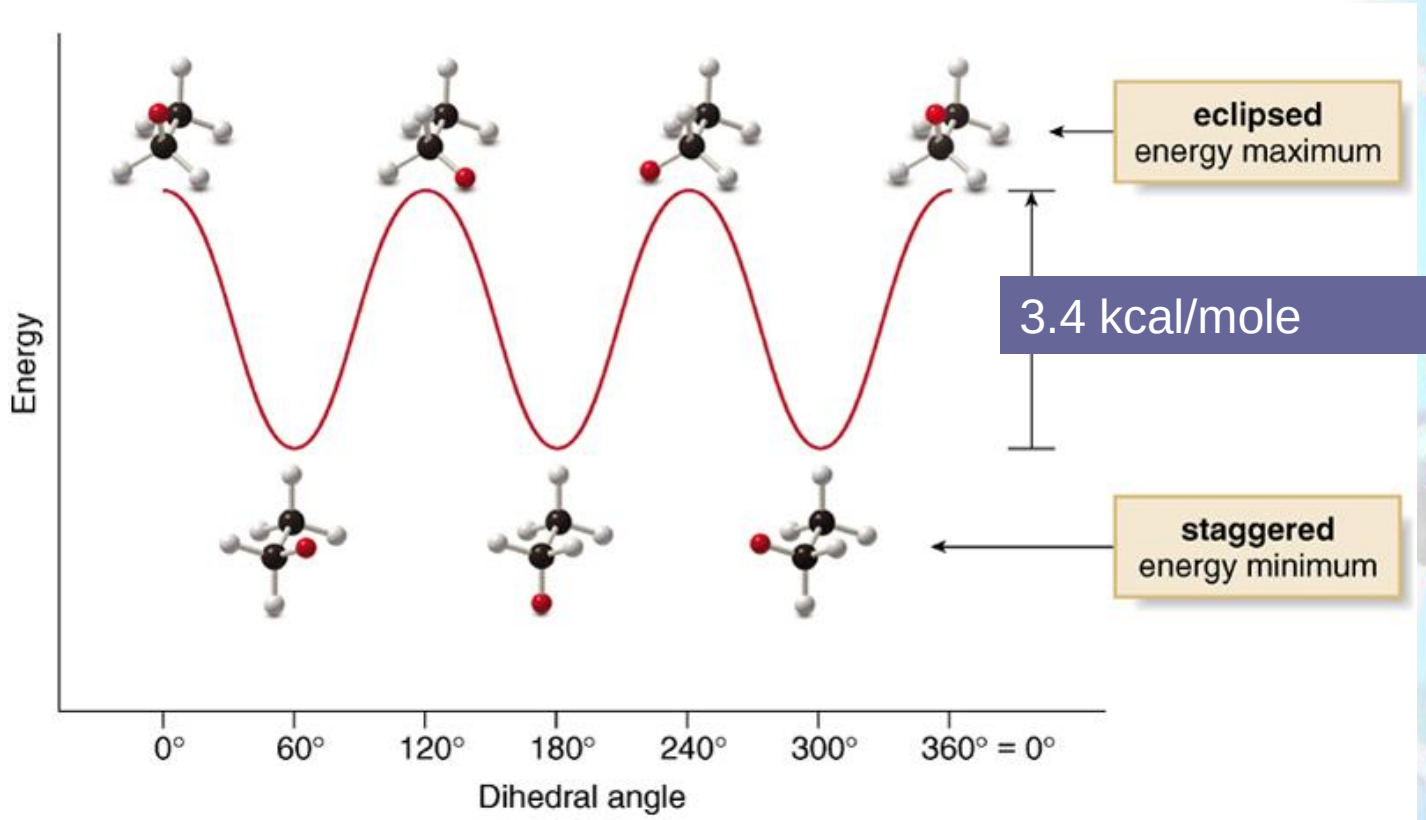


Propane

- Torsional barrier is 14 kJ/mol (3.4 kcal/mol)
- Eclipsed conformation has three interactions
  - Two ethane-type hydrogen-hydrogen interactions
  - One additional hydrogen-methyl interaction

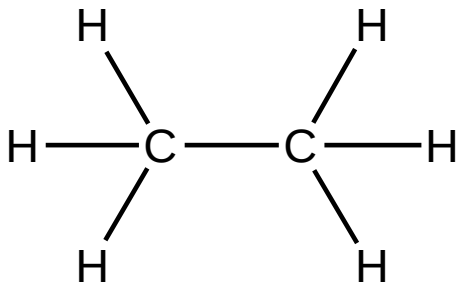


Graph: Energy versus dihedral angle for Propane

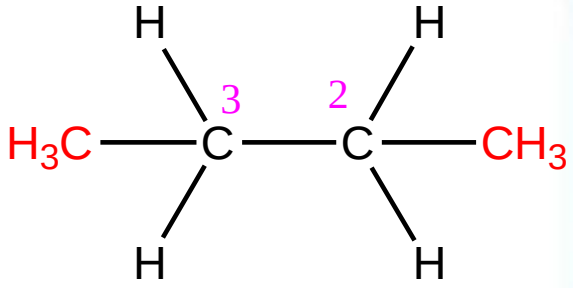


تحليل الهيئة لجزئ البيوتان
Conformation Butane

ذكرنا من قبل أن الجزئ الموجود في تشكيل ما يمكن ان يوجد في أكثر من هيئة نتيجة الدوران الحر حول الرابطة الأحادية.
فمثلا إذا اعتبرنا جزي بيوتان و ركزنا انتباهنا على الدوران حول الرابطة C(2)- C(3) فإننا نحصل على عدة هيئات يتوقف عددها على زاوية الدوران. و لتسهيل تصور تلك الهيئات سنستخدم صيغة نيومان (Newman)
لتمثيل تلك الهيئات و نفحص نتيجة دوران 60º أو مضاعفاتها حتى نصل إلى زاوية دوران 360º



Ethane



Butane

- An energy minimum and maximum occur every 60° as the conformation changes from staggered to eclipsed. Conformations that are neither staggered nor eclipsed are intermediate in energy.
- Butane and higher molecular weight alkanes have several C—C bonds, all capable of rotation. It takes six 60°

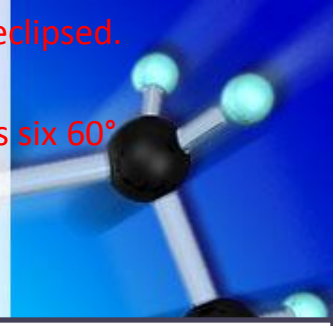
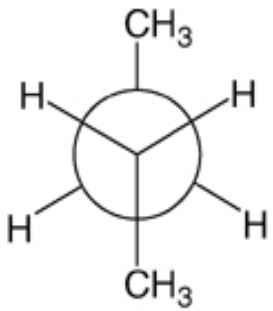


Figure :



1

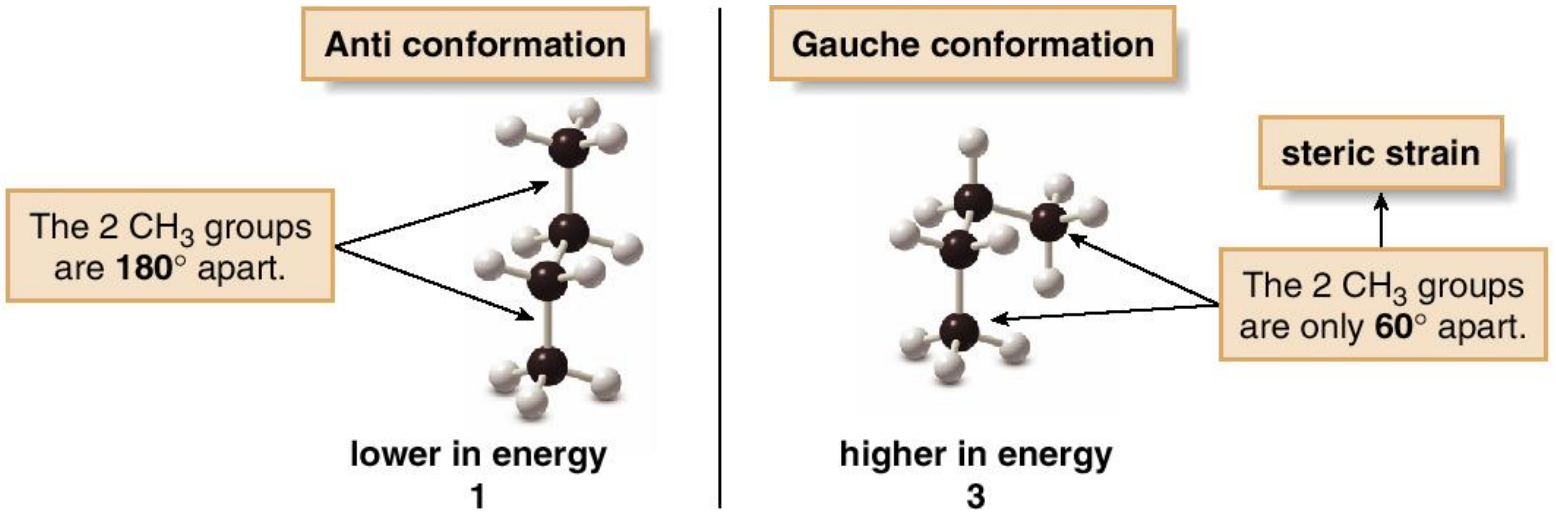
staggered, anti

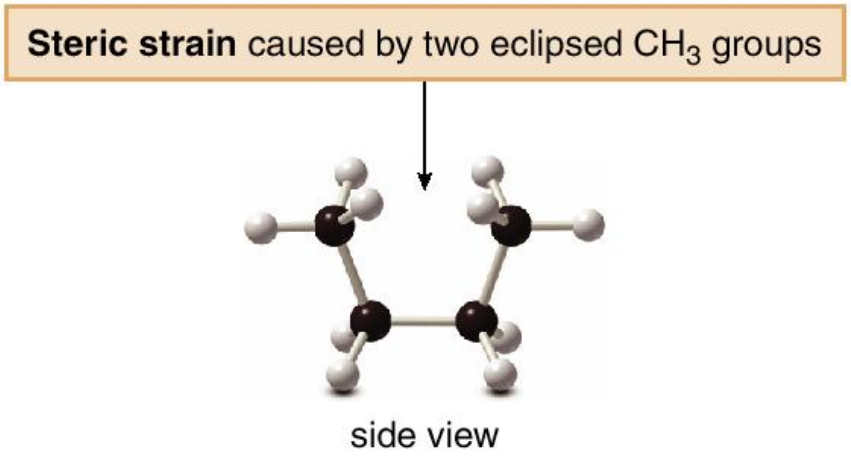
متعاقبة ـ مضادة

- A staggered conformation with two larger groups 180° from each other is called anti.
- A staggered conformation with two larger groups 60° from each other is called gauche.
- The staggered conformations are lower in energy than the eclipsed conformations.
- The relative energies of the individual staggered conformations depend on their steric strain.
- Steric strain is an increase in energy resulting when atoms are forced too close to one another.
- Gauche conformations are generally higher in energy than anti conformations because of steric

التشكيل المتعاقب - المضاد
الزاوية 180 - اقل طاقة

المتعاقب – جوش
الزاوية 60





الوضع المنكسف اعلى طاقة – بسبب التنافر بين مجاميع الميثل

Figure:

دراسة منحى الطاقة للبيوتان

- Staggered conformations **1, 3,** and **5** are at energy minima.
- Anti conformation **1** is lower in energy than gauche conformations **3** and **5,** which possess steric strain.
- Eclipsed conformations **2, 4,** and **6** are at energy maxima.
- Eclipsed conformation **4,** which has additional steric strain due to two eclipsed CH_3 groups, is highest in energy.

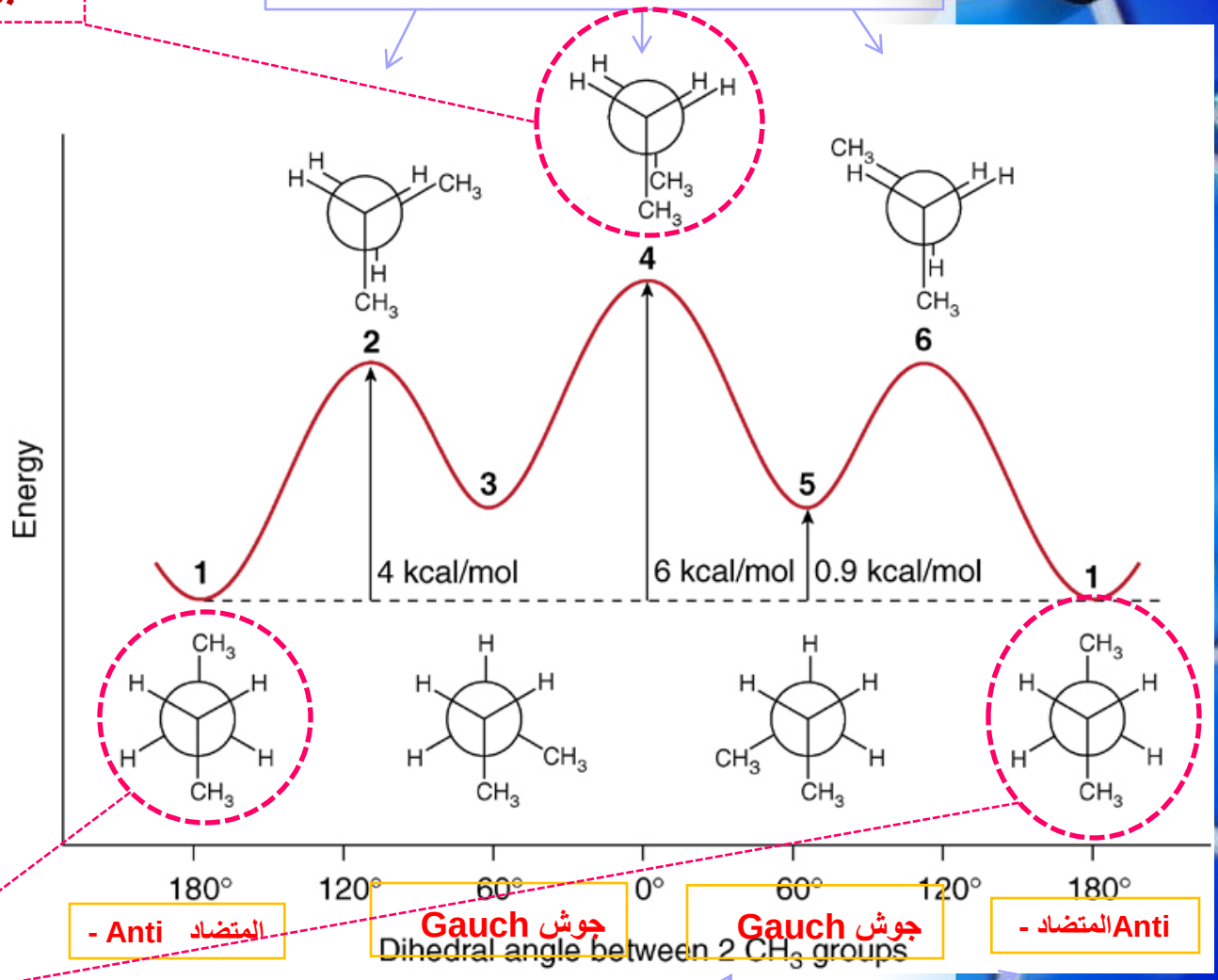


Table 4.3 Summary: Torsional and Steric Strain Energies in Acyclic Alkanes

Type of interaction	Energy increase (kcal/mol)
H,H eclipsing	1
H,CH_3 eclipsing	1.5
CH_3,CH_3 eclipsing	4
gauche CH_3 groups	0.9

- The energy difference between the lowest and highest energy conformations is called a barrier to rotation.
- Since the lowest energy conformation has all bonds staggered and all large groups anti, alkanes are often drawn in zigzag skeletal structures to indicate

A zigzag arrangement keeps all carbons **staggered** and **anti**.