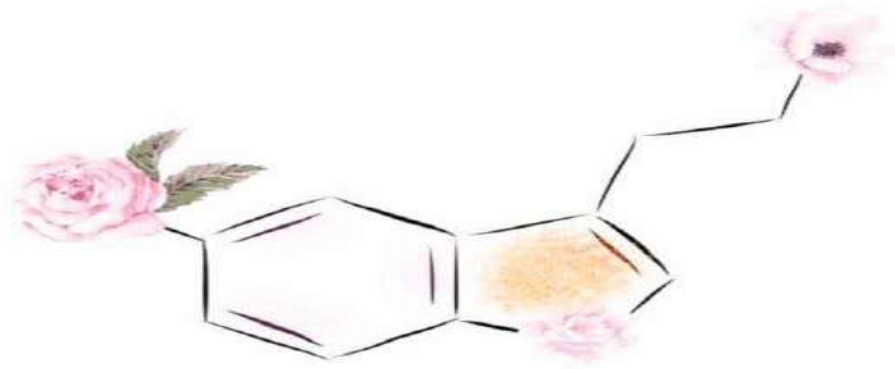


Date: 27/10/2023



لجان الدفقات



## تفريغ عضويه 1

موضوع المحاضرة: Chapter ( 1 )

رقم المحاضرة: ( 3 + 4 )

إعداد الصيدلانيه: Gufran Khaseeb



### Nomenclature

0 Most organic compounds are known by two or more names:

- The older unsystematic names, (*Common* → شائعة)
- The *IUPAC* names. ← Before

International Union of Pure & Appplied Chemistry

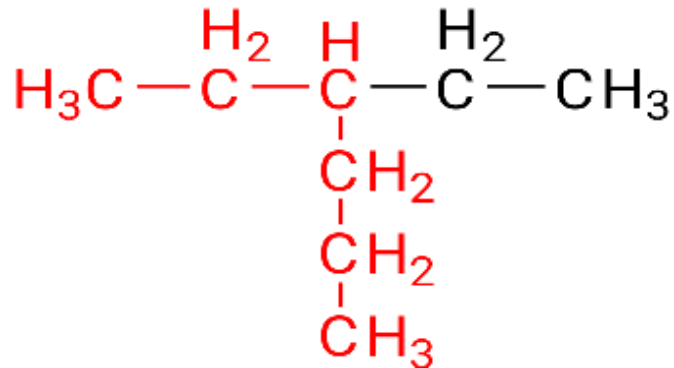
# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

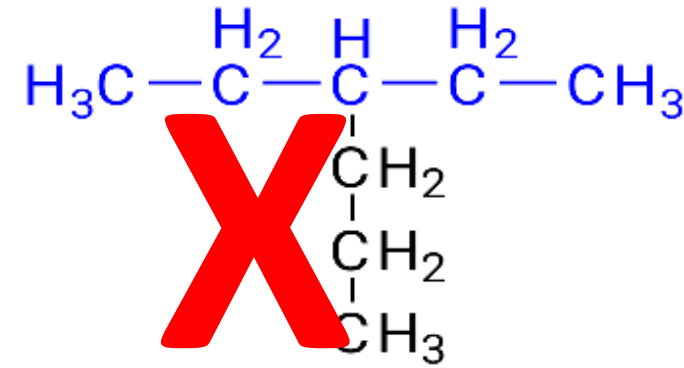
#### The IUPAC Rules

- 1 Select the parent structure =  
the longest continuous chain



2 6  
Ethyl hexane

ضايفينوا عليه (منكتبه قبله)



not

Propyl pentane

The longest continuous chain is not necessarily straight. <sup>سقيمة</sup>reason: the bond used (sigma) have free rotation <sup>single</sup>

ممكن يكون المركب مائل و هو straight

# Saturated Hydrocarbons

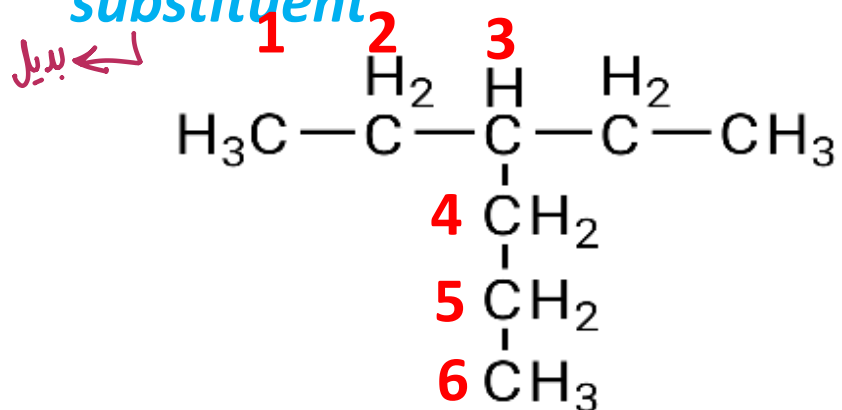
## 1. Alkanes

### Nomenclature

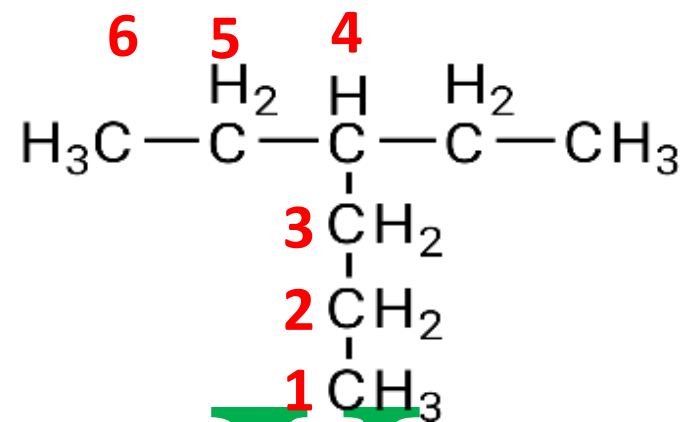
### The IUPAC Rules

② Number the carbons in the parent chain

*starting from the end which gives the lowest number for the substituent*



3-Ethyl hexane



4-Ethyl hexane

**X**

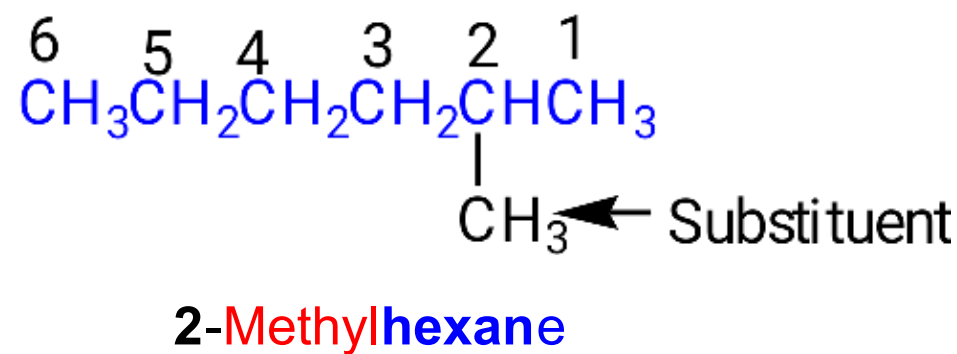
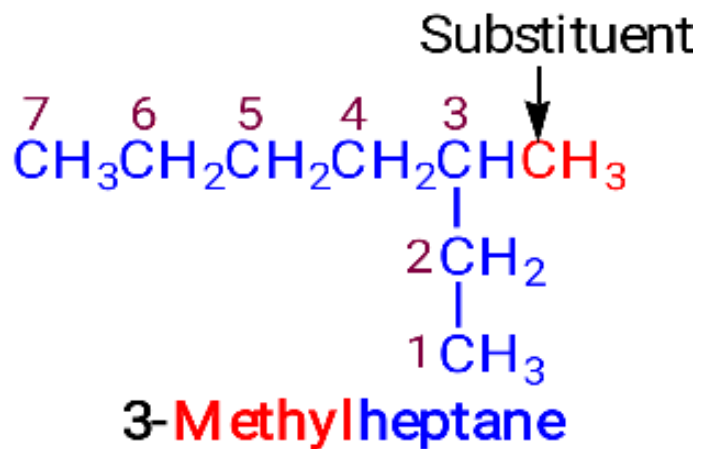
# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

### The IUPAC Rules

2) Number the carbons in the parent chain



### Nomenclature

#### The IUPAC Rules

To name the compound;

- 1) The position of the substituent on the parent carbon chain by a number.
- 2) The number is followed by a hyphen (-).
- 3) The combined name of the substituent (ethyl).
- 4) The parent carbon chain (hexane)

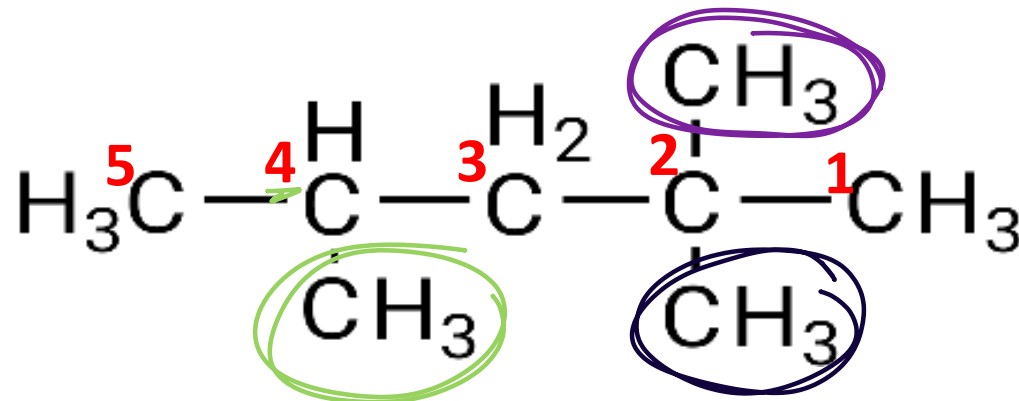
# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

### The IUPAC Rules

- ③ If the **same alkyl substituent** occurs more than once on the parent carbon chain, the prefixes <sup>(2)</sup>di-, <sup>(3)</sup>tri-, <sup>(4)</sup>tetra-, <sup>(5)</sup>penta-, and so on are used to indicate **two**, **three**, **four**, **five**, and so on.



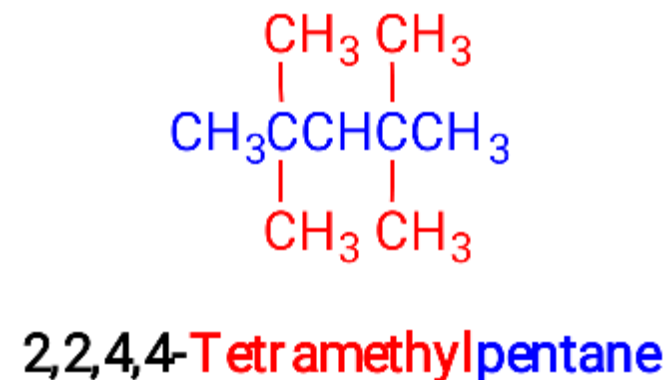
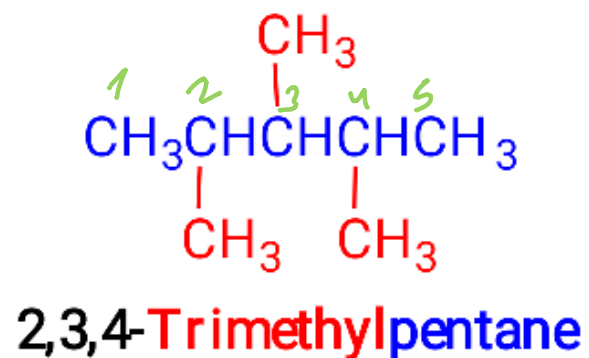
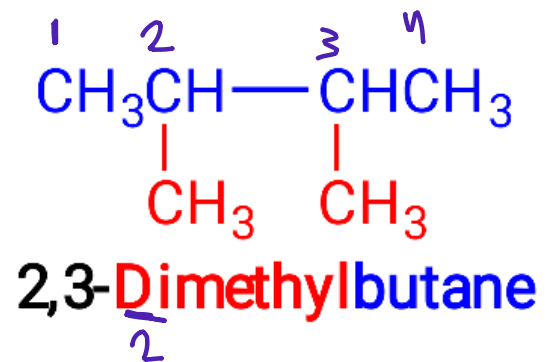
**2,2,4-Tri methylpentane**

# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

### The IUPAC Rules



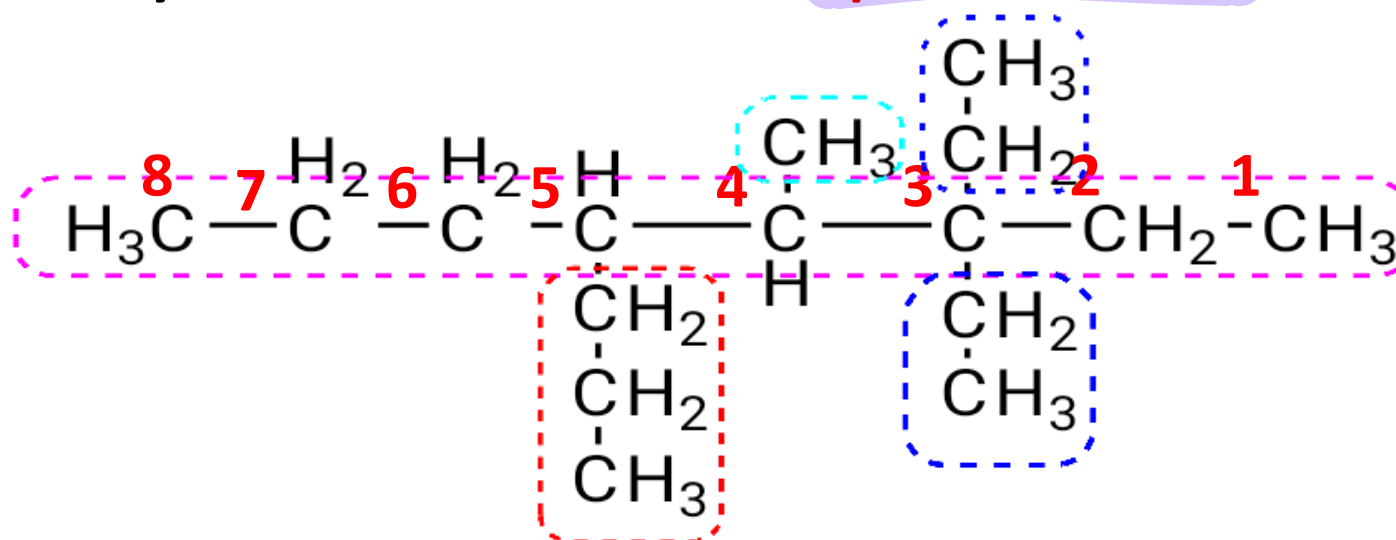
# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

### The IUPAC Rules

- 4) If **different alkyl substituents** are attached on the parent carbon chain, they are named in order of **alphabetical order**.



3,3- di ethyl  
4- methyl  
5- propyl

**3,3-Diethyl -4-methyl- 5-propyl octane**

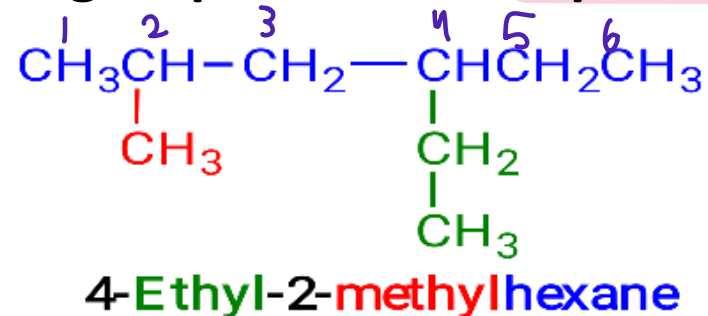
# Saturated Hydrocarbons

## 1. Alkanes

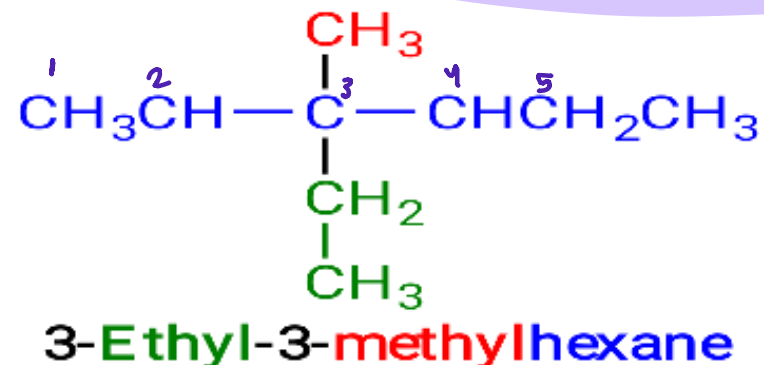
### Nomenclature

#### The IUPAC Rules

**Note** that each substituent is given a number corresponding to its location on the longest chain. The substituent groups are listed **alphabetically**.



5) When **two substituent** are present on the same carbon, **use the number twice**.



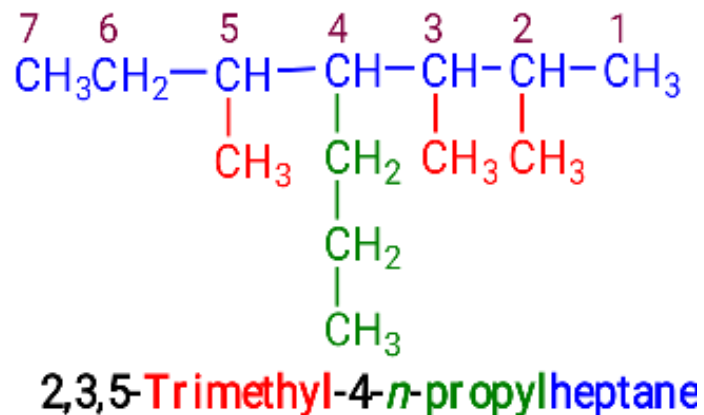
# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

### The IUPAC Rules

- 6) When two chains of equal length compete for selection as the parent chain, choose the chain with the greater number of substituents.



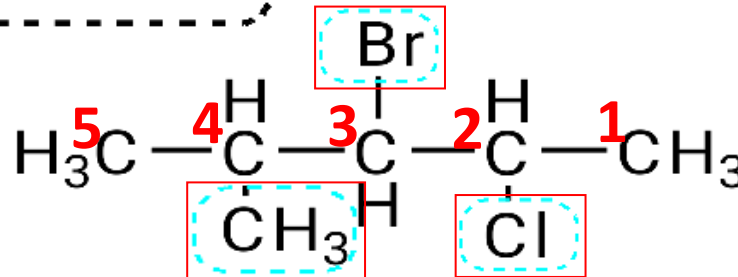
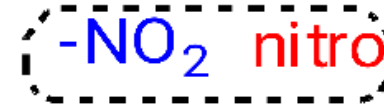
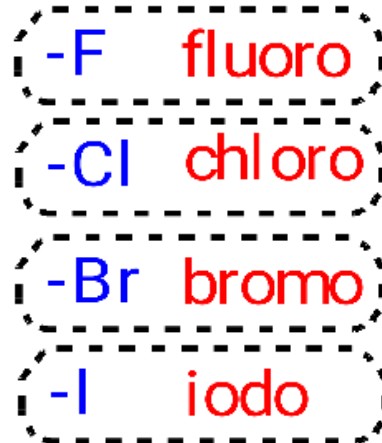
# Saturated Hydrocarbons

## 1. Alkanes

### Nomenclature

### The IUPAC Rules

- ⑦ If **substituents other than alkyl groups** are also present on the **parent carbon chain**; **all substituents are named alphabetically.** الأولوية إلهم



2-chloro  
3-bromo  
4-methyl

3-bromo -2-chloro -4-methylpentane

## 1. Alkanes

### Sources of Alkanes

0 The two principal sources of alkanes are **petroleum** and **natural gas**.

Petroleum and natural gas constitute the chief sources of

- Alkanes up to 40 Carbons

- Aromatic (Gasoline and its derivatives)

- ~~Alicyclic~~ (Cyclic aliphatic hydrocarbons) (Alicyclic) [saturated]

- Heterocyclic Unsaturated (x atoms (N,O,S))

# Saturated Hydrocarbons

## 1. Alkanes

### Sources of Alkanes

### Petroleum Refining

Some components of refined petroleum

| Fraction                                               | Boiling range (°C) | Carbon content |
|--------------------------------------------------------|--------------------|----------------|
| Gas quickly evaporates                                 | Below 20           | C1 – C4        |
| Petroleum ether                                        | 20 – 60            | C5 – C6        |
| Naphtha                                                | 60 – 100           | C6 – C7        |
| Gasoline                                               | 40 – 200           | C5 – C10       |
| Kerosine                                               | 175 – 325          | C11 – C18      |
| Gas oil                                                | 300 – 500          | C15 – C40      |
| Lubricating oil, asphalt, petroleum coke and paraffins | Above 400          | C15 – C40      |

↑ number of carbon ÷ ↓ Boiling Point

gas → liquid → solid

greasy ← compounds

# Saturated Hydrocarbons

## 1. Alkanes

### Physical Properties

### Physical Properties of Alkanes, Alkenes and Alkynes

Those properties that can be observed without the compound undergoing a chemical reaction

#### A. Physical States

C1 (C2) to C4 are gases,

C5 to C17 are liquids,

C18 and larger alkanes are wax <sup>(semi)</sup> -like solids.

2 layers  
└─ dissolved (2 layers disappeared)  
   not (2 layers didn't disappear)

#### B. Solubility

- Alkanes, Alkenes and Alkynes are **nonpolar** compounds. → H  
composed of  
→ O
- Their solubility “**Like dissolve like**”
- Alkanes, Alkenes and Alkynes are **soluble** in the **nonpolar solvents**;  
**carbon tetrachloride, CCl<sub>4</sub> and benzene,**
- Alkanes, Alkenes and Alkynes are **insoluble** in **polar solvents** like **water**.

# Intermolecular Forces and Liquids and Solids

# Intermolecular Forces (To know the nature of the material)

① **Intermolecular forces** are attractive forces between (different) molecules.

② **Intramolecular forces** hold atoms together in a molecule.

## Intermolecular vs Intramolecular

- 41 kJ to vaporize 1 mole of water (inter) (weaker)
- 930 kJ to break all O-H bonds in 1 mole of water (intra) (stronger)

multiple choice question

## "Measure" of intermolecular force

boiling point

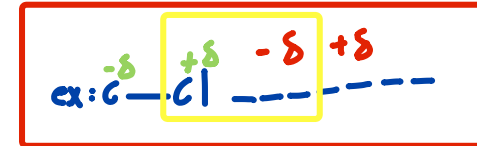
melting point

Generally, **intermolecular** forces are much weaker than **intramolecular** forces.

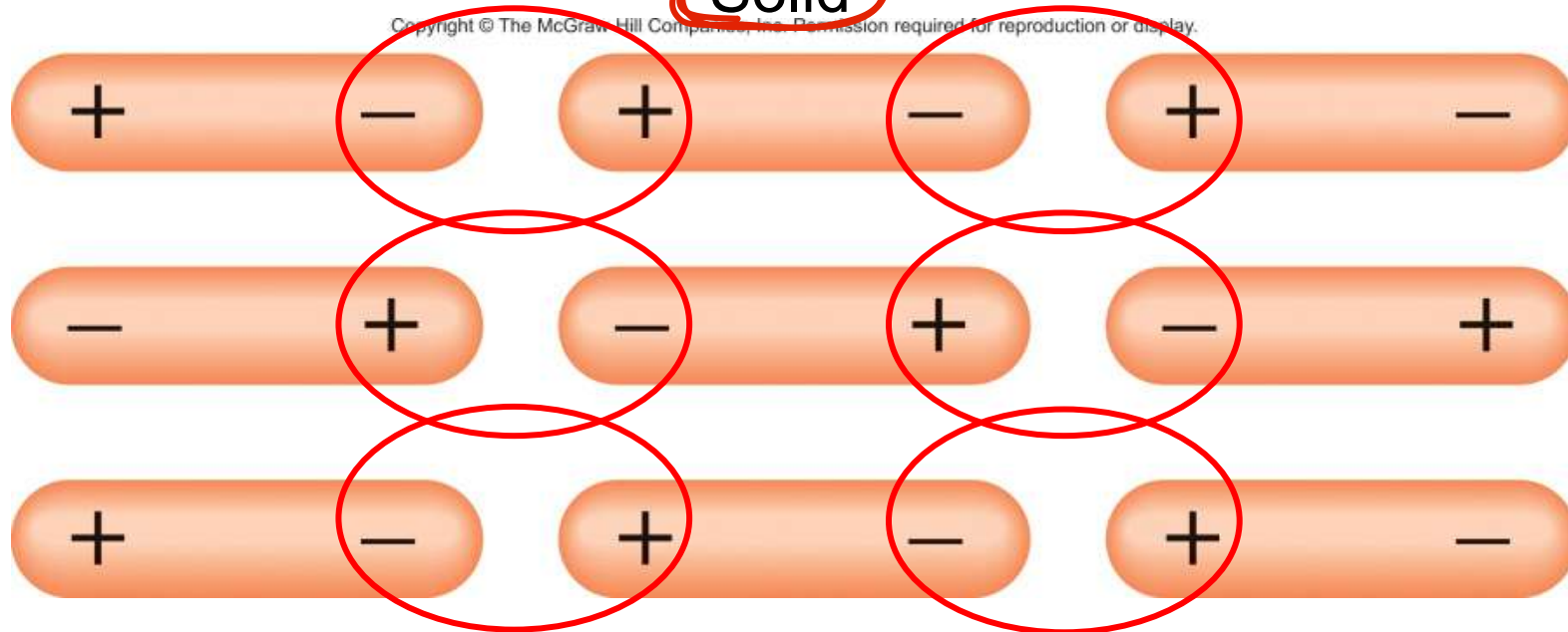
# Intermolecular Forces

## Dipole-Dipole Forces

Attractive forces between polar molecules



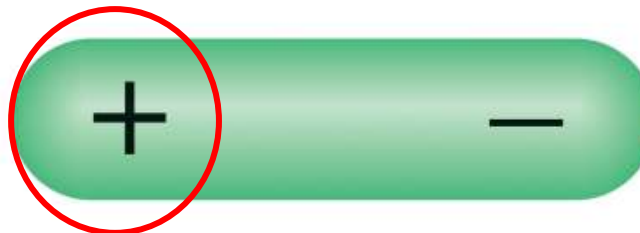
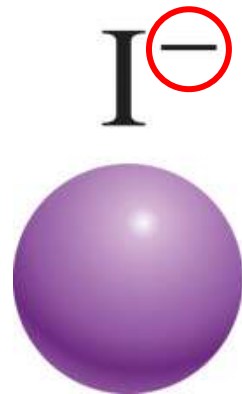
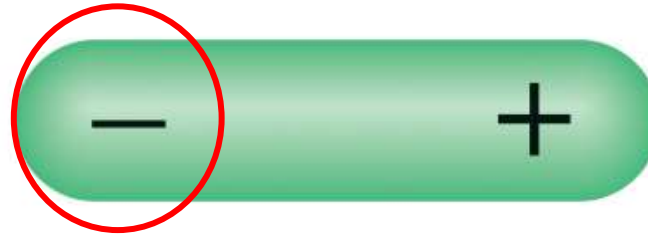
Orientation of Polar Molecules in a  
Solid



# Intermolecular Forces

Attractive forces between an ion and a polar molecule

## Ion-Dipole Interaction



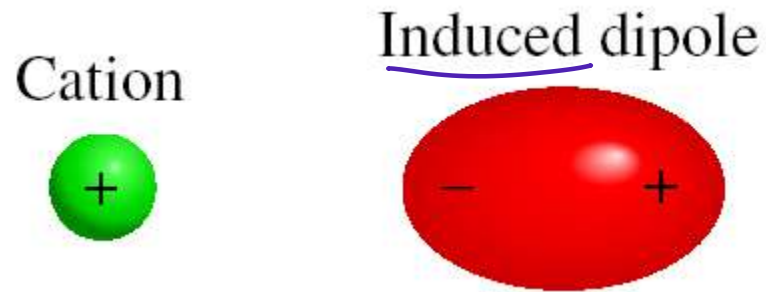
# London forces (dipole-induced dipole attraction)

- Non-polar molecules do not have dipoles like polar molecules. How, then, can non-polar compounds form solids or liquids?
- London forces (also called van der Waal forces) are due to small dipoles that exist in non-polar molecules
- Because electrons are moving around in atoms there will be instants when the charge around an atom is not symmetrical
- The resulting tiny dipoles cause attractions between atoms/molecules (the greater the mass, the greater the London forces)

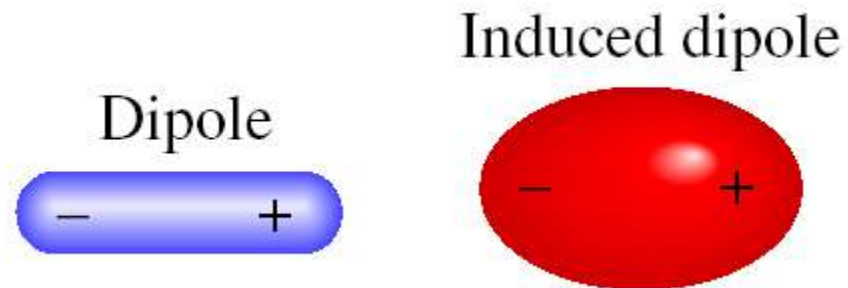
# Intermolecular Forces

## Dispersion Forces

Attractive forces that arise as a result of **temporary dipoles induced** in atoms or molecules



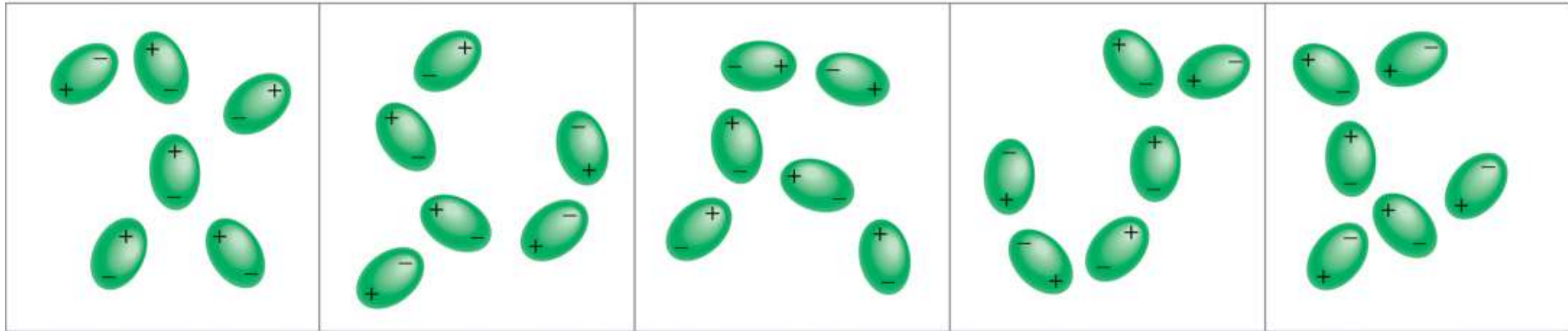
ion-induced dipole interaction



dipole-induced dipole interaction

# Induced Dipoles Interacting With Each Other

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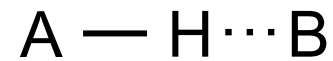


# Intermolecular Forces

## Hydrogen Bond

Is very important for soluble in  
*polar* ← solvents or not

The **hydrogen bond** is a special dipole-dipole interaction between the hydrogen atom in a polar N-H, O-H, or F-H bond and an electronegative O, N, or F atom.

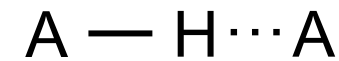


*6 group*

*5 group*

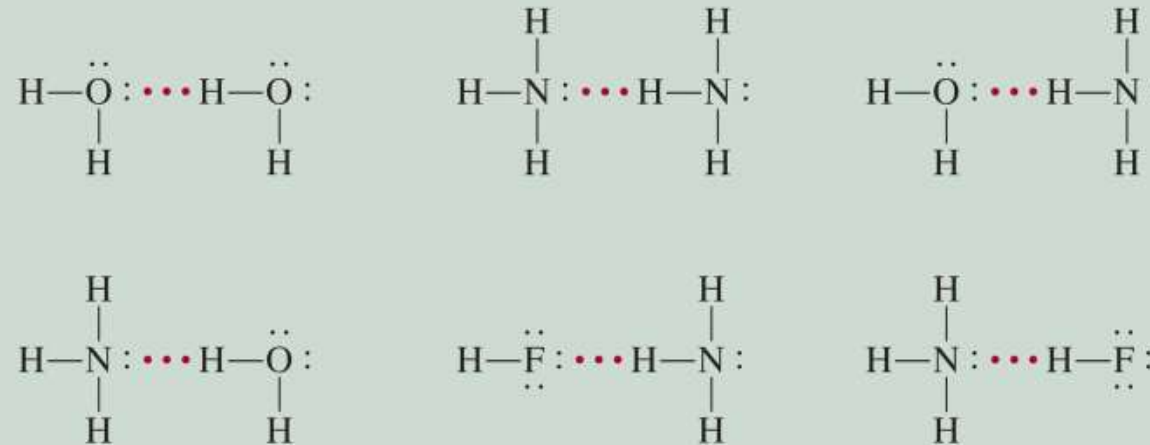
*7 (group 7)*

O



A & B are N, O, or F

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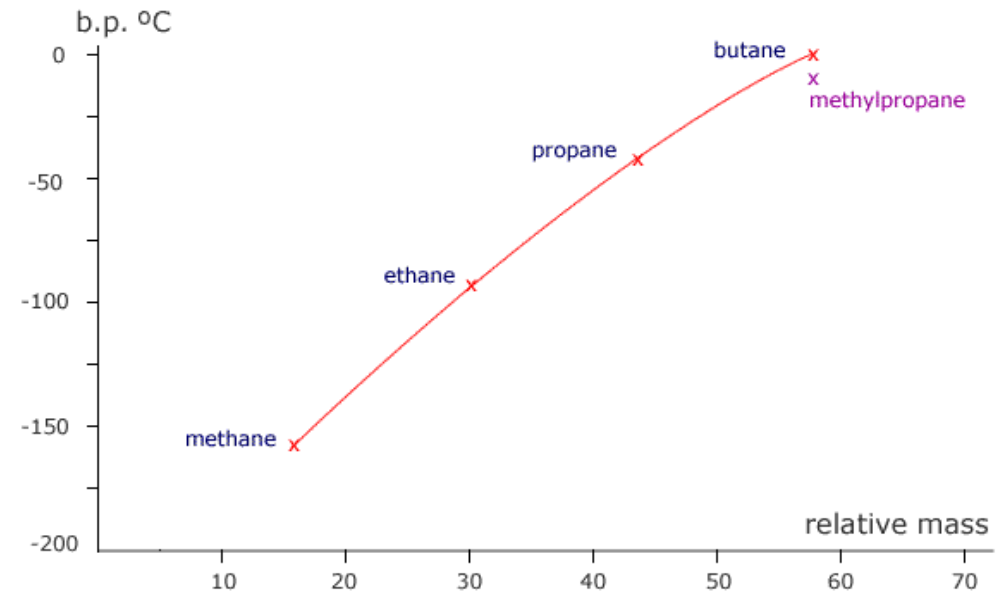
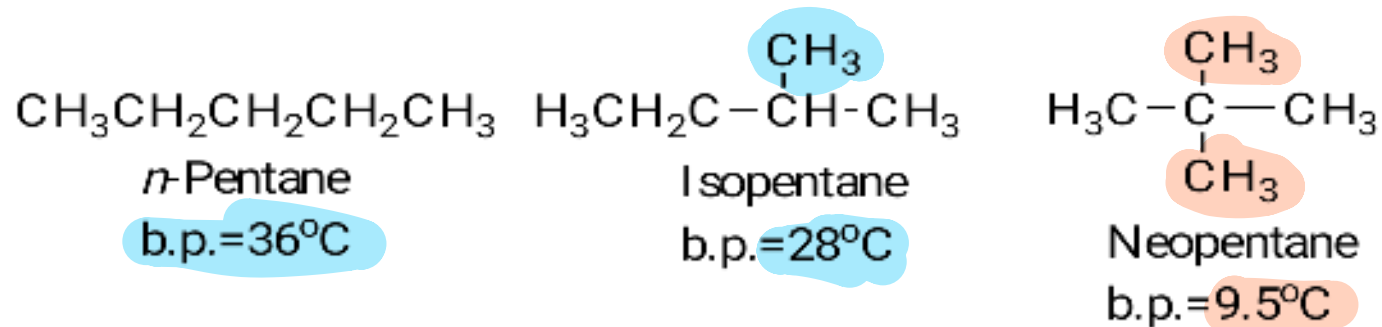
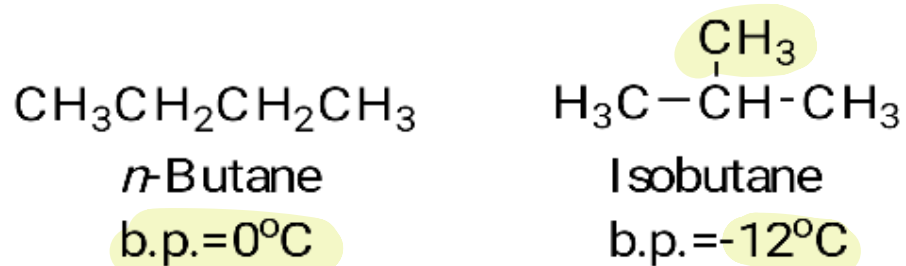


# Saturated Hydrocarbons

## 1. Alkanes

### Physical Properties

### C. Boiling Points



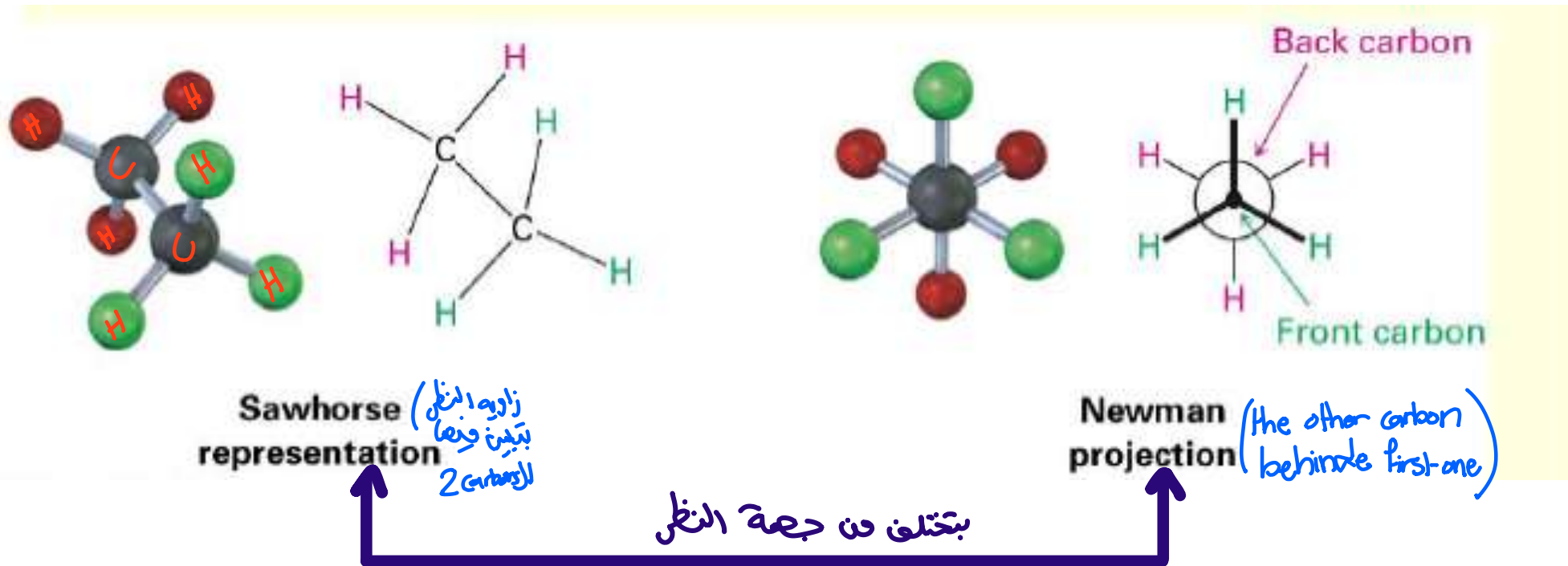
Graph showing boiling point of the alkanes against relative mass

- Boiling point decreases with increasing branches
- Boiling point increases with increasing molecular weight.

# Conformational Isomers of

## Alkanes

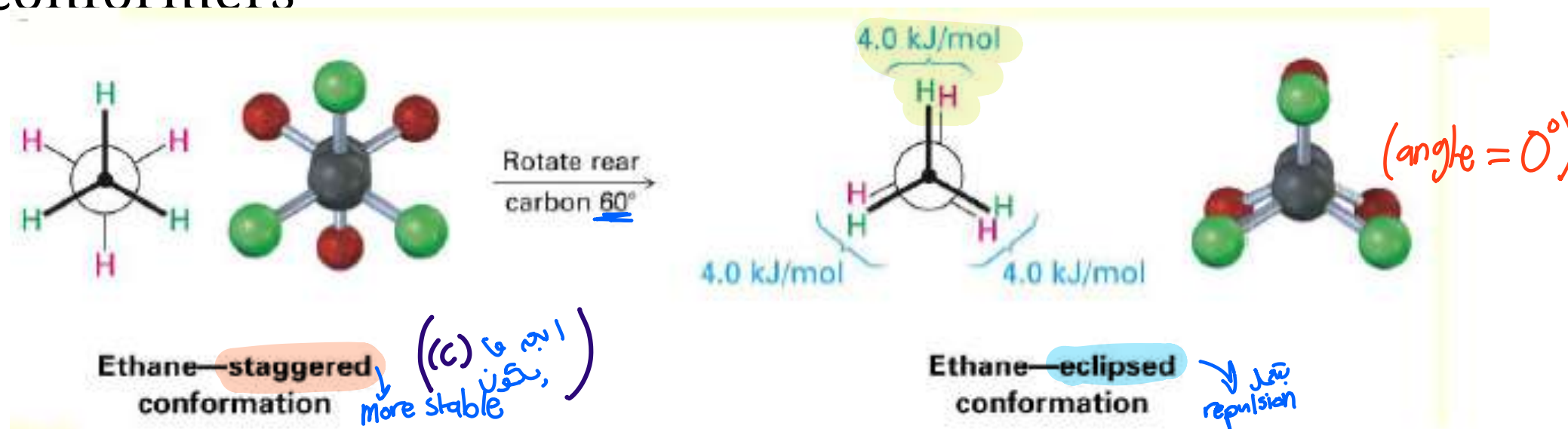
Isomers that differ as a result of sigma bond  
Isomers that differ as a result of sigma bond  
rotation of C-C bond in alkanes



# Bond Rotation and Newman

## Projections

As carbon-carbon bond rotates, interconvert carbon bond rotates, interconvert between staggered and eclipsed conformers



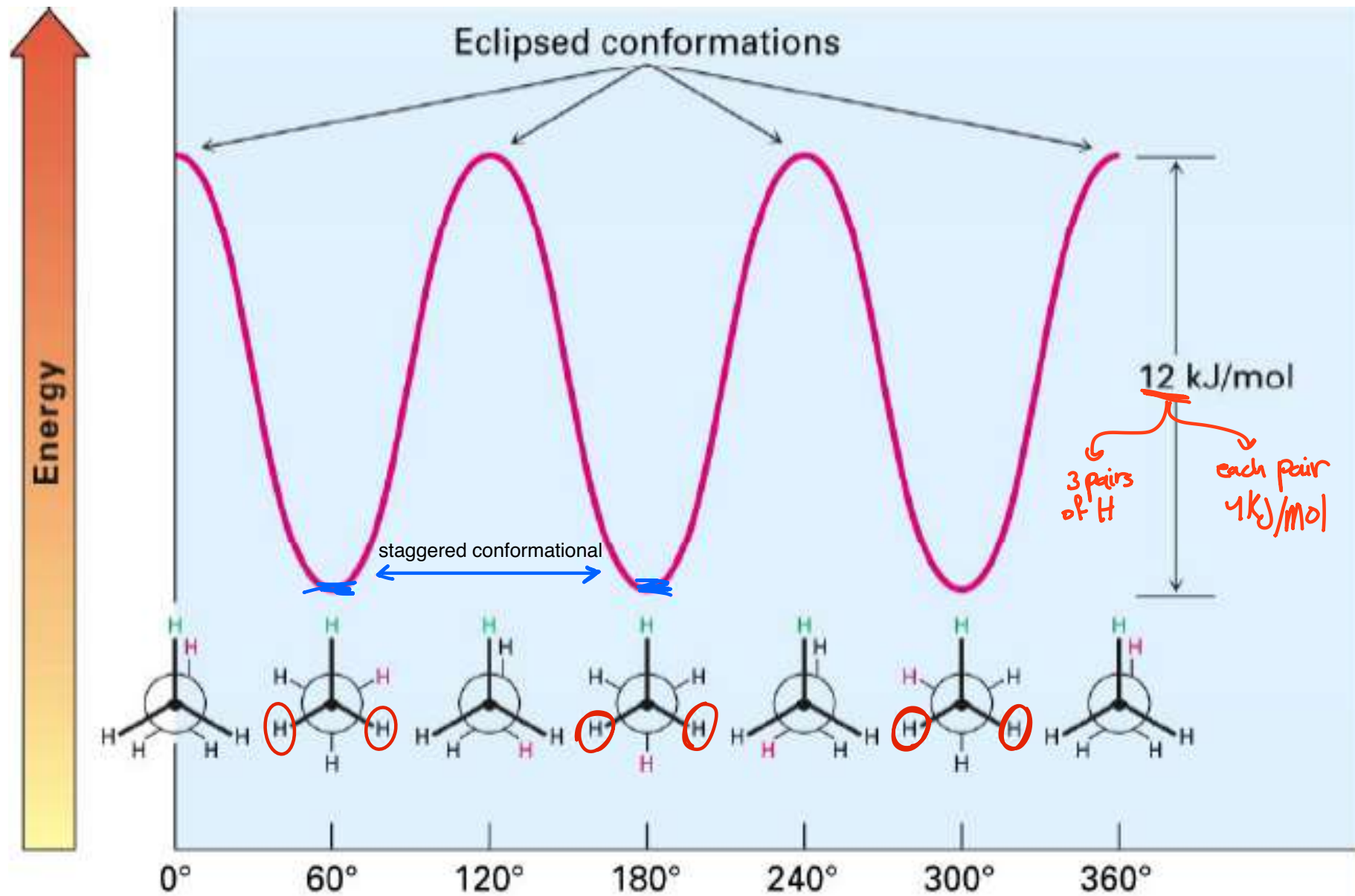
Eclipsed conformer is 12.0 kJ/mol higher in energy ('free' rotation at room temperature)

# Repulsion <sup>يؤذي</sup> → <sup>طاقة الاجهاد الالتوائي</sup> Torsional Strain Energy

Force that <sup>يعارض</sup> opposes rotation due to the repulsion Force that opposes rotation due to the repulsion of bonding electrons

- We do not observe perfectly free rotation
- There is a <sup>حاجز</sup> barrier to rotation, and some conformers are more stable than others
- Small energy barrier easily overcome at RT
- Each eclipsed H-H costs 4 kJ/mol of Torsional Energy

→ in staggered  
الرجاء ما يكون (H)  
عند راحة  
less energy  
in stable situation  
(60°, 180°, 300°)



# Strain Energy in Alkanes

## Torsional Strain

Steric strain- repulsive interaction occurring between atoms that are forced closer together than their at far from each other.

**Table 3.5** | Energy Costs for Interactions in Alkane Conformers

| Interaction                                | Cause                       | Energy cost |            |
|--------------------------------------------|-----------------------------|-------------|------------|
|                                            |                             | (kJ/mol)    | (kcal/mol) |
| H ↔ H eclipsed                             | Torsional strain            | 4.0         | 1.0        |
| H ↔ CH <sub>3</sub> eclipsed               | Mostly torsional strain     | 6.0         | 1.4        |
| CH <sub>3</sub> ↔ CH <sub>3</sub> eclipsed | Torsional and steric strain | 11          | 2.6        |
| CH <sub>3</sub> ↔ CH <sub>3</sub> gauche   | Steric strain               | 3.8         | 0.9        |

تقریباً منہ بجھ  
بس منہ ورا بجھ

# Saturated Hydrocarbons

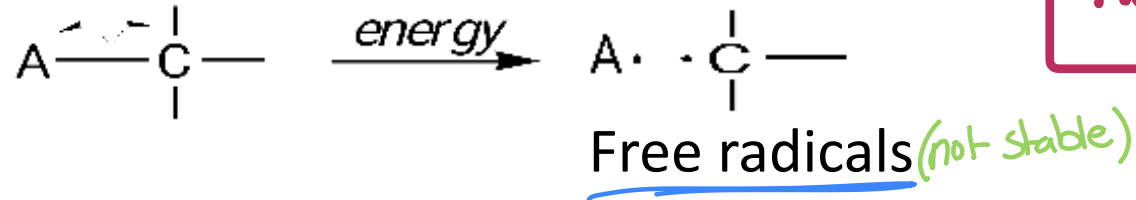
## 1. Alkanes

### Notations for bond breaking and bond making

0 A covalent bond can be broken in either two ways,

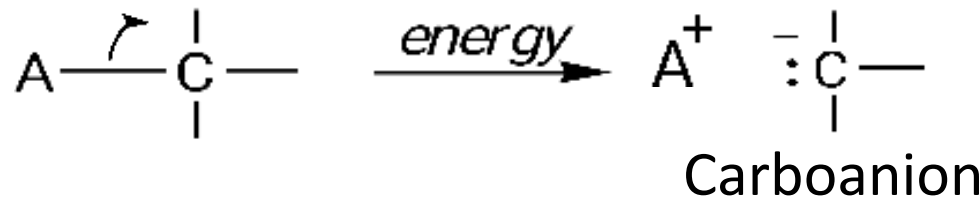
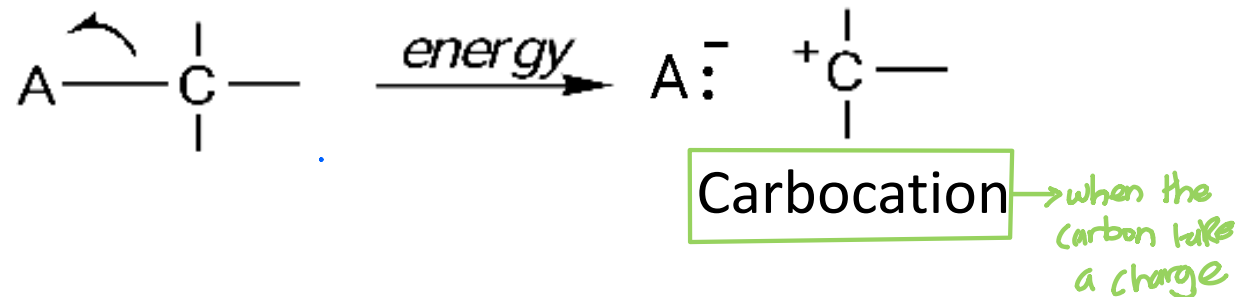
□ Homolytic cleavage.

كل واحد يأخذ الإلكترون  
تتبعو



□ Heterolytic cleavage.

one of the molecules take charge  
the another one  
Positively charged



the homolytic need high energy than heterolytic

# Saturated Hydrocarbons

## 1. Alkanes

### Preparation of Alkanes

*(adding a H to a compound)*

#### 1) Hydrogenation of Alkenes and Alkynes

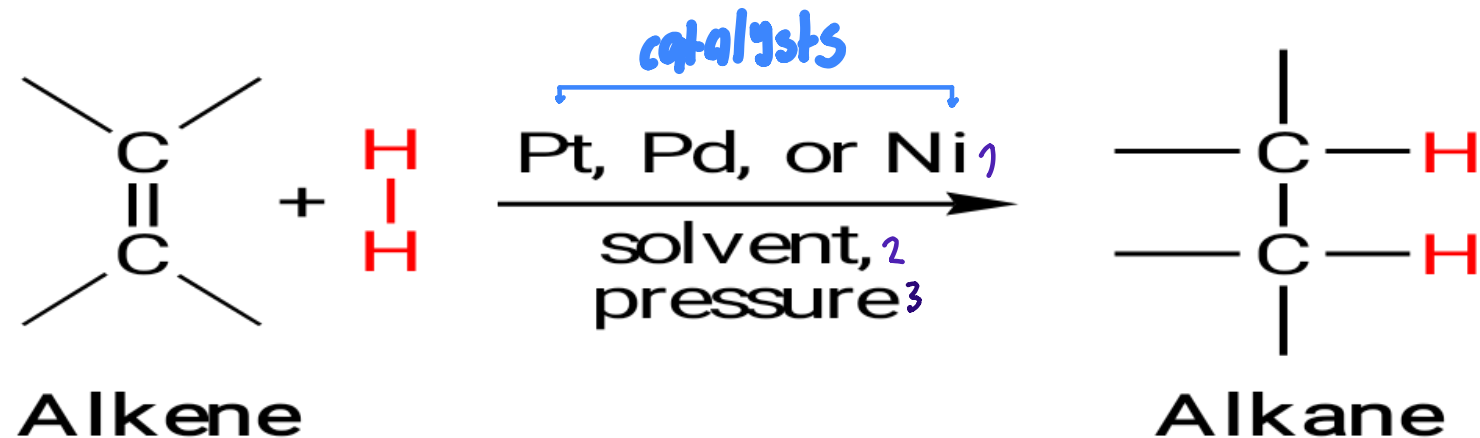
A great number of alkanes can be obtained by fractional distillation of crude petroleum and subsequent reactions as follows:

*the main source  
(natural)*

##### 1. Catalytic hydrogenation: *in the lab*

*Alkenes and alkynes* react with hydrogen in the presence of **metal catalysts** such as nickel, palladium, and platinum to produce alkanes.

##### General Reaction

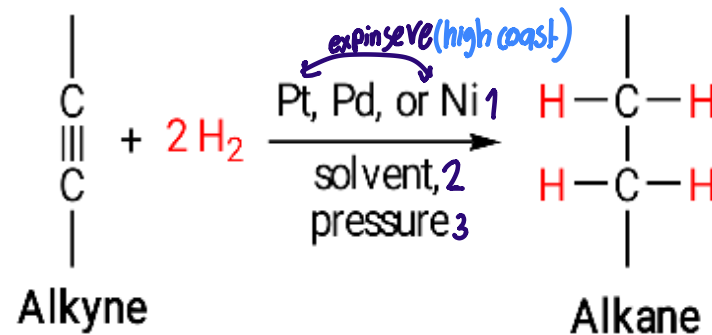


# Saturated Hydrocarbons

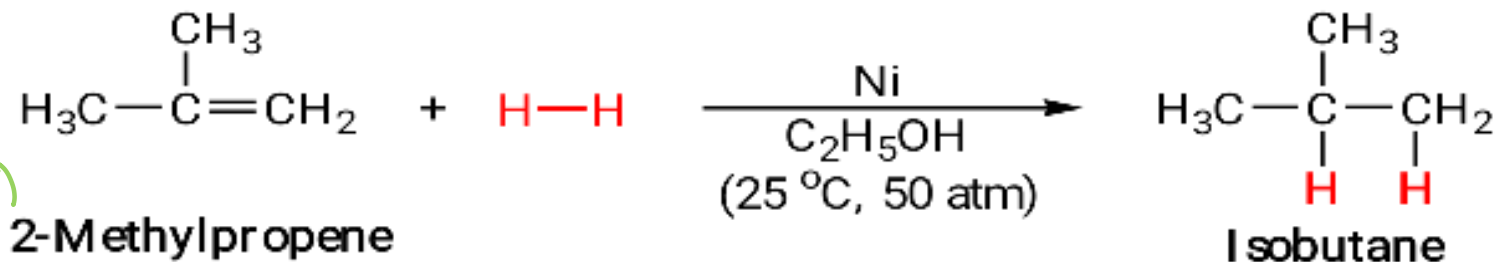
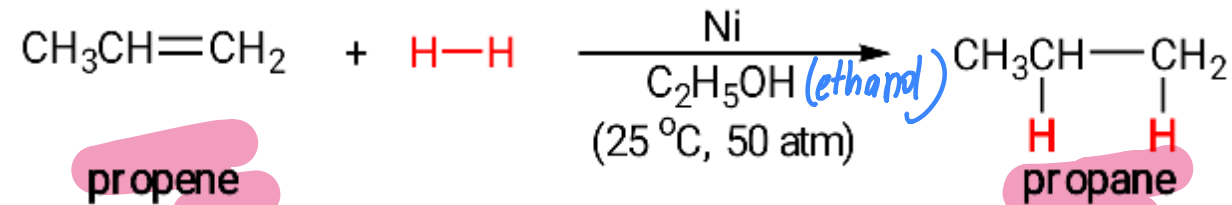
## 1. Alkanes

### Preparation of Alkanes

#### 1) Hydrogenation of Alkenes and Alkynes



#### o Specific Examples

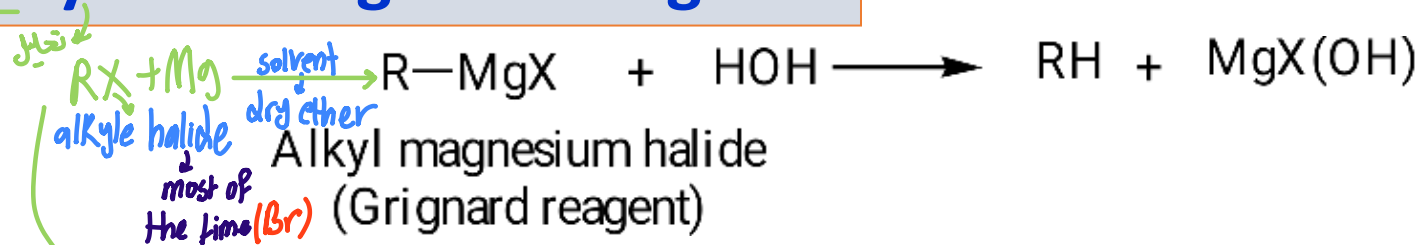


# Saturated Hydrocarbons

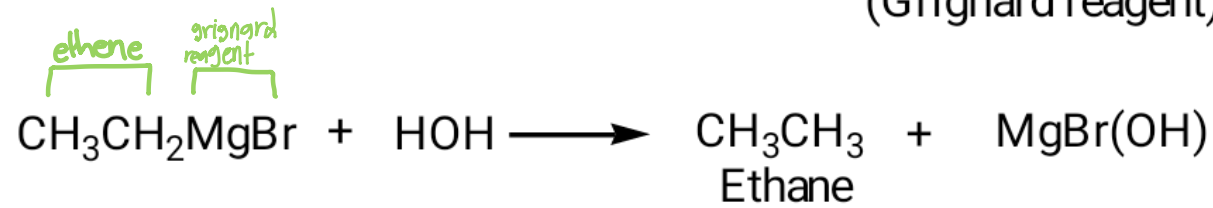
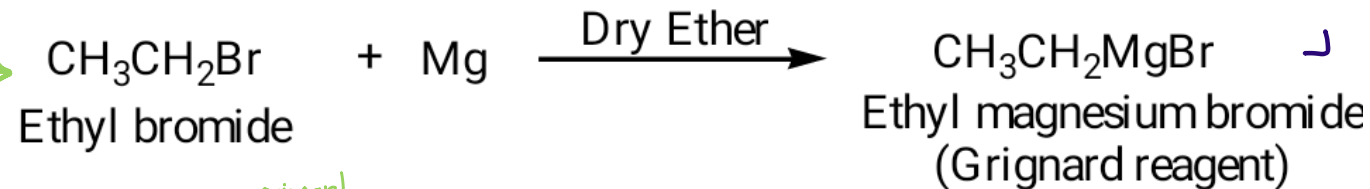
## 1. Alkanes

### Preparation of Alkanes

#### 2) <sup>H<sub>2</sub>O</sup>Hydrolysis of Grignard Reagent



**O Grignard reagents** react readily with any source of protons to give hydrocarbons.



#### 3) By coupling of alkyl halides with dialkyl cuprate (all kinds of alkanes)



# Saturated Hydrocarbons

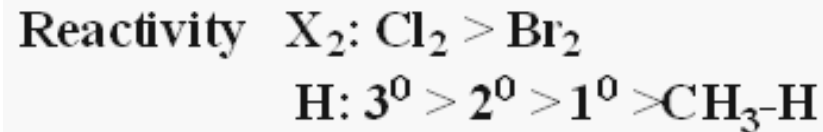
## 1. Alkanes

### Reactions of Alkanes

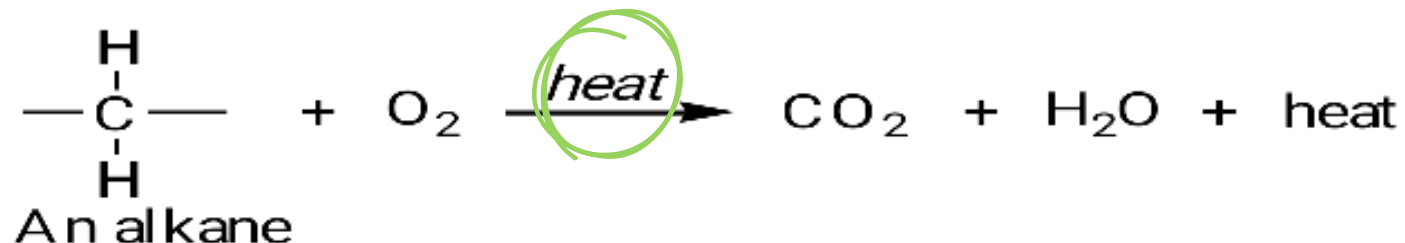
Saturated hydrocarbons undergo very few reactions, so they are called **Paraffinic hydrocarbons**. (Latin *parum*, little; *affinis*, affinity)

### Halogenation

The **halogenation** of an alkane appears to be a simple free radical substitution in which a C-H bond is broken and a new C-X bond is formed



### Combustion



### Reactions of Alkanes

#### A. Halogenation

○ Substitution reaction of alkanes,

استبدال

i.e. replacement of hydrogen by halogen,

usually chlorine or bromine, giving alkyl chloride or alkyl bromide.

○ Flourine reacts explosively with alkanes

It is unsuitable reagent for the preparation of the alkyl flourides. (highly reactive) (the most electronegative)

○ Iodine is too unreactive

It is not used in the halogentaion of alkanes.

○ Halogenation of alkanes take place at

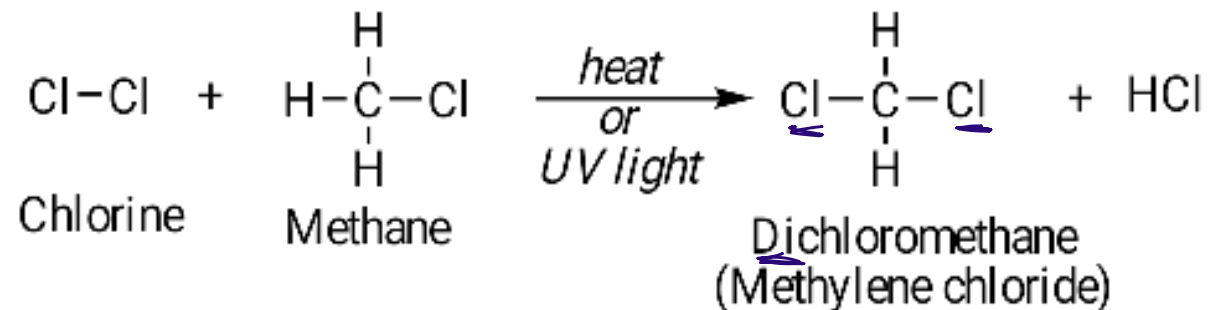
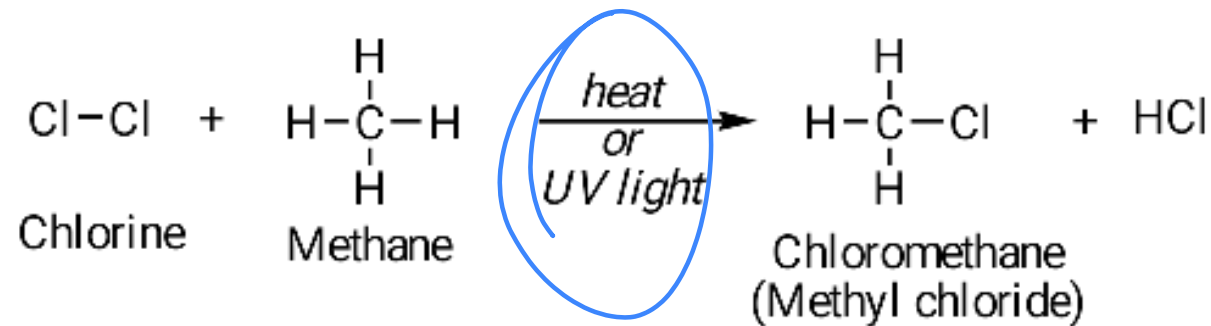
high temperatures or under the influence of ultraviolet light

## 1. Alkanes

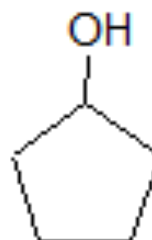
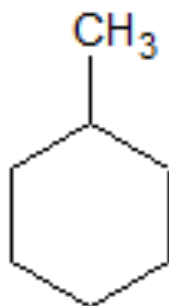
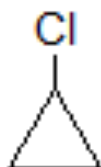
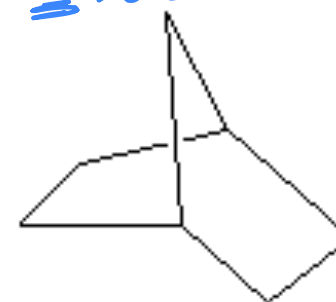
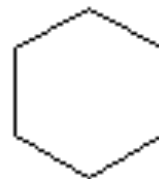
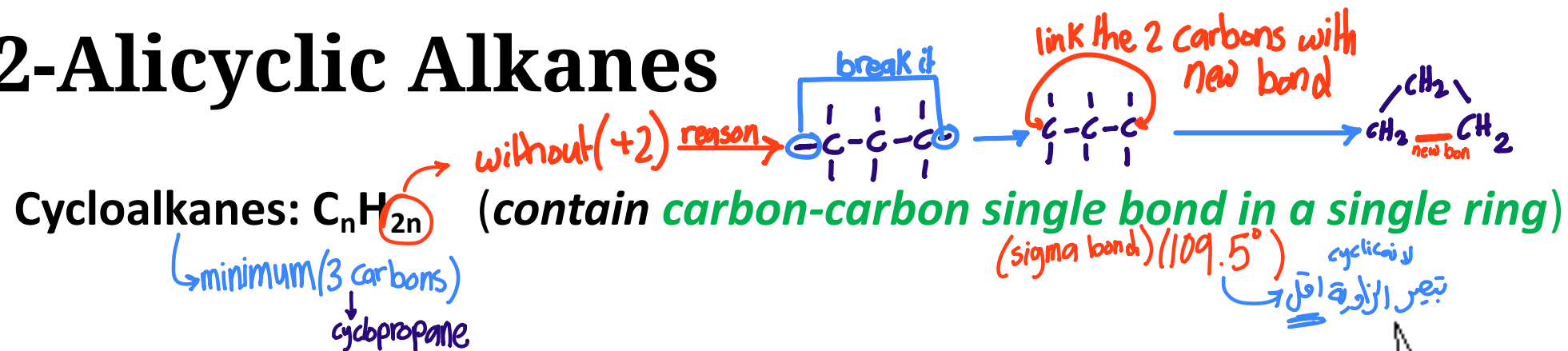
### Reactions of Alkanes

#### A. Halogenation

- o Chlorination of an alkane usually gives a mixture of products <sup>at any reaction</sup> { price → sheep  
multiple product  
isolation → it costs money and time



# 2-Alicyclic Alkanes

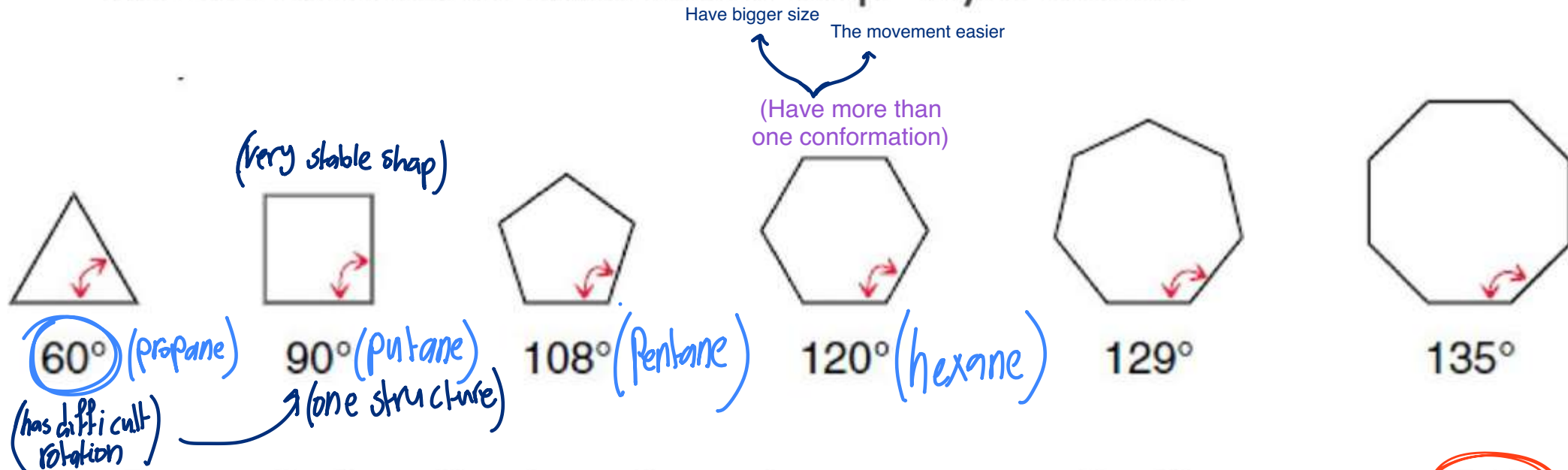


# Saturated Hydrocarbons

## 2. Alicyclic Alkanes

### Cyclic Alkanes

- Carbon atoms in alkanes are  $sp^3$  hybridized



- To optimize the bond angles, most cycloalkanes are **NOT** **flat** in their **most stable conformation**

- Alkanes with closed ring(s) of C atoms
- General formula:  $C_nH_{2n}$  ( $C_3H_6$ ,  $C_4H_8$ ,  $C_5H_{10}$ , etc.)
- Naming:** use **cyclo-** prefix before alkane name



(one structure)

**cyclo**propane

$n = 3$

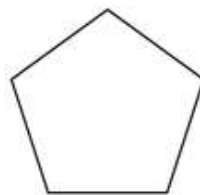
$C_3H_6$



**cyclo**butane

$n = 4$

$C_4H_8$



more than one conformation

**cyclo**pentane

$n = 5$

$C_5H_{10}$



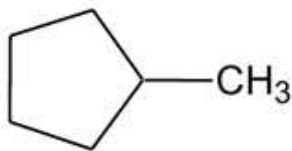
**cyclo**hexane

$n = 6$

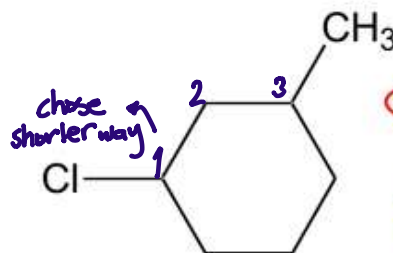
$C_6H_{12}$

Naming substituted cycloalkanes:

- 1 substituent: no numbering necessary
- 2 or more substituents: highest alpha priority on C #1



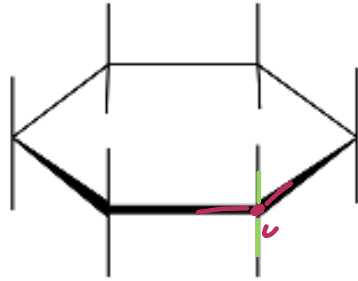
methylcyclopentane



~~1-chloro-5-methylcyclohexane~~

1-chloro-3-methylcyclohexane

# Conformations of Cyclohexane

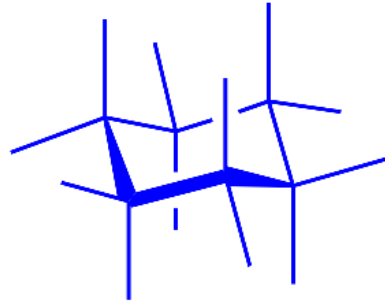


Cyclohexane does not have any angle strain! It isn't a flat molecule. By rotating about the carbon-carbon bonds, it can achieve  $109.5^\circ$  bond angles.

the substituents (in the C)   
 → axial (up) (down)   
 → equatorial

(The form is **un**less diverse)

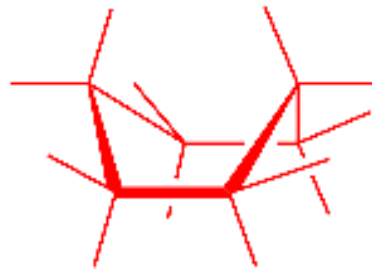
# conformations of cyclohexane



chair

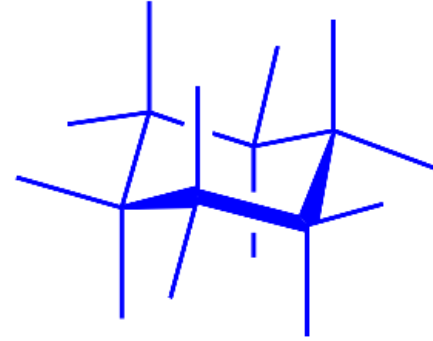
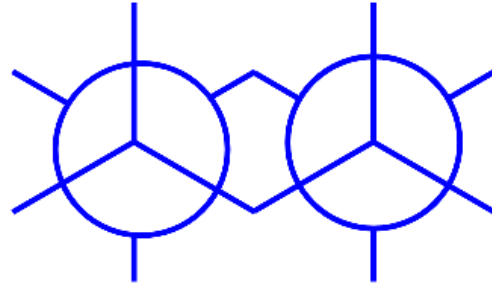


twist boat



boat

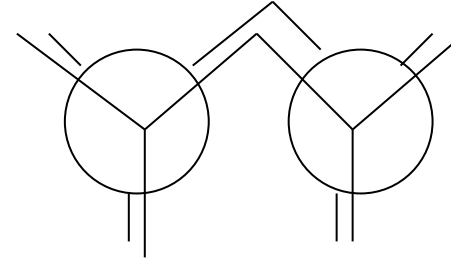
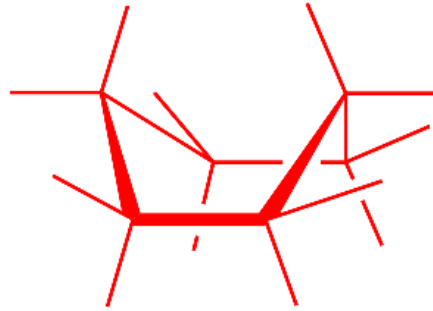
# conformations of cyclohexane



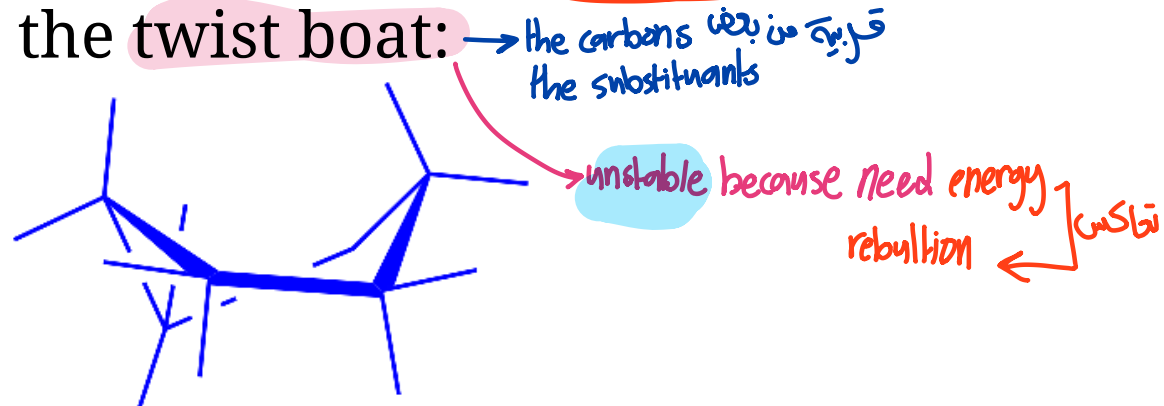
The **chair** conformation of cyclohexane is free of both angle strain and torsional strain (deviation from staggered). **This is the most stable conformation.**

→ the substituents ابن ما يركن  
+ the carbons

# conformations of cyclohexane



The boat conformation is free of angle strain, but has a great deal of torsional strain (eclipsed). To relieve the strain, it twists slightly to form the twist boat:



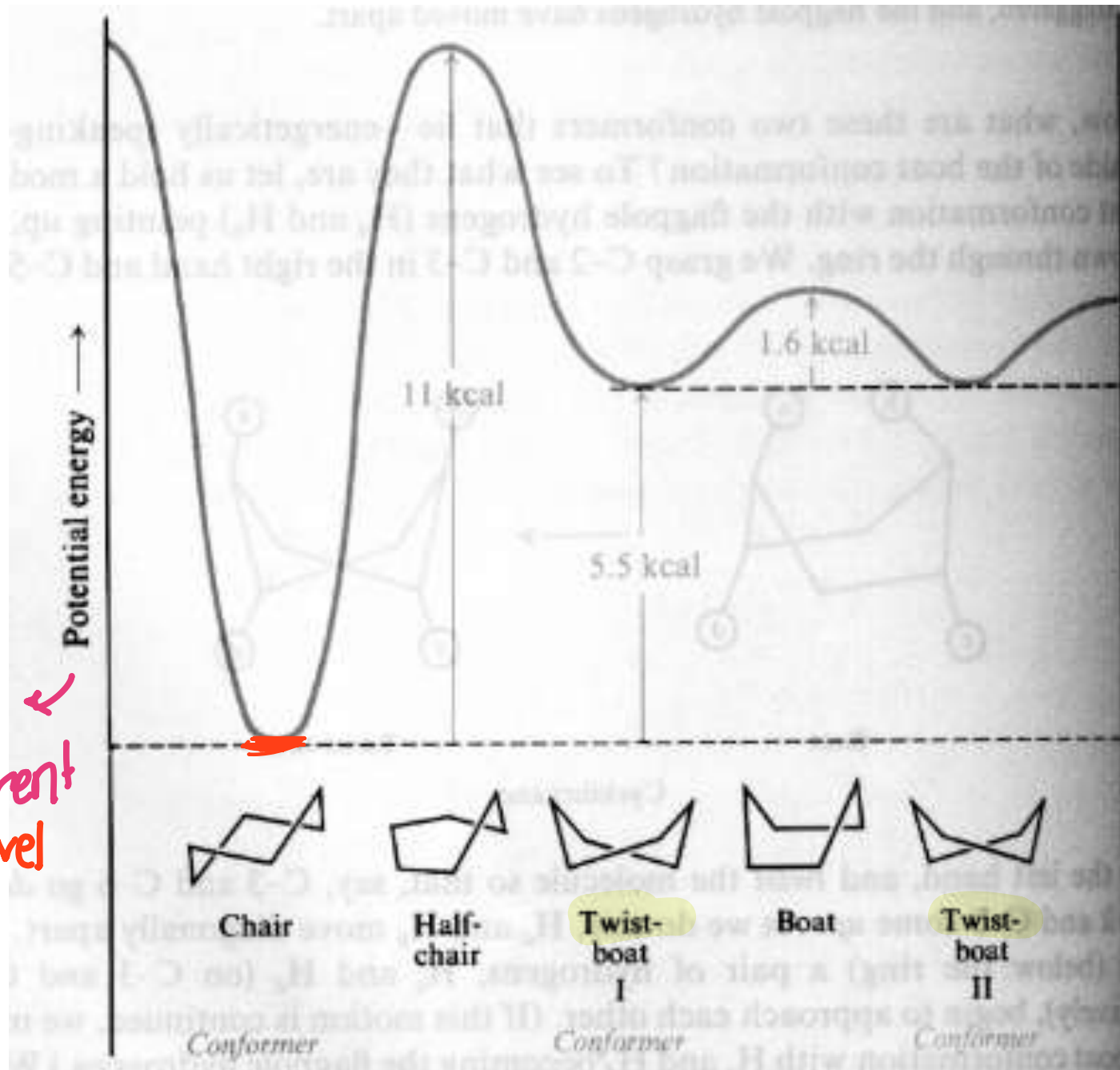
# conformations of cyclohexane

الزمن 360°  
في الشكل  
Chair & boat في.

most popular shapes  $\left\{ \begin{array}{l} \text{cyclohexane} \\ \text{cyclopentane} \end{array} \right.$

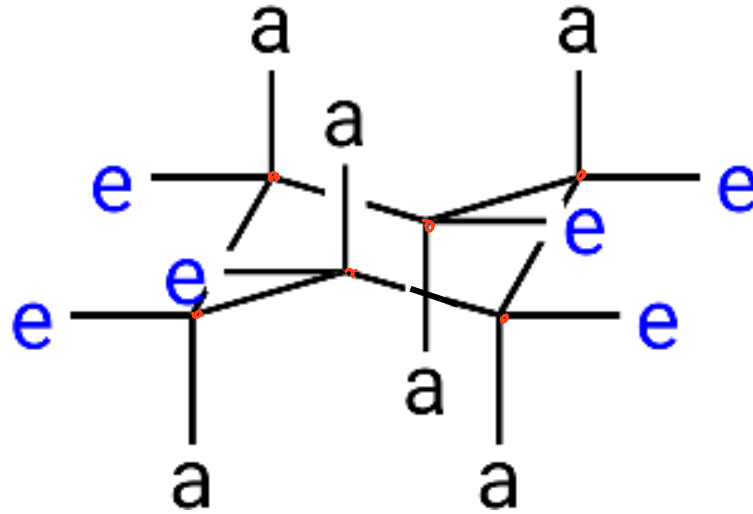
The most stable  
the least energy

every one  $\leftarrow$   
have different  
energy level



# conformations of cyclohexane

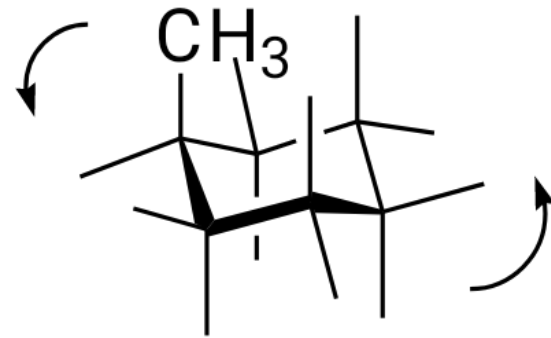
6 carbons (12 substituents)



a = <sup>عمودية</sup> axial positions in the chair conformation

e = <sup>افقية</sup> equatorial positions

# conformations of cyclohexane

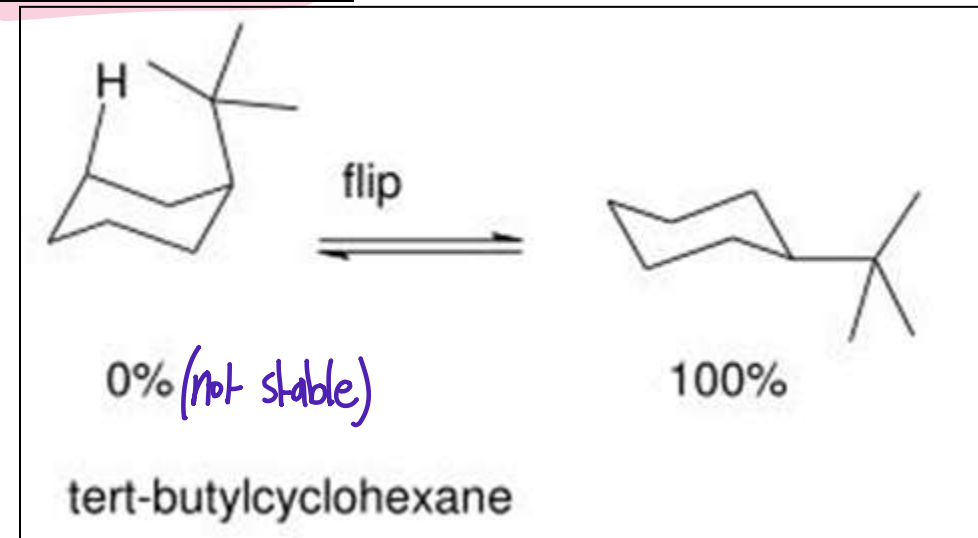
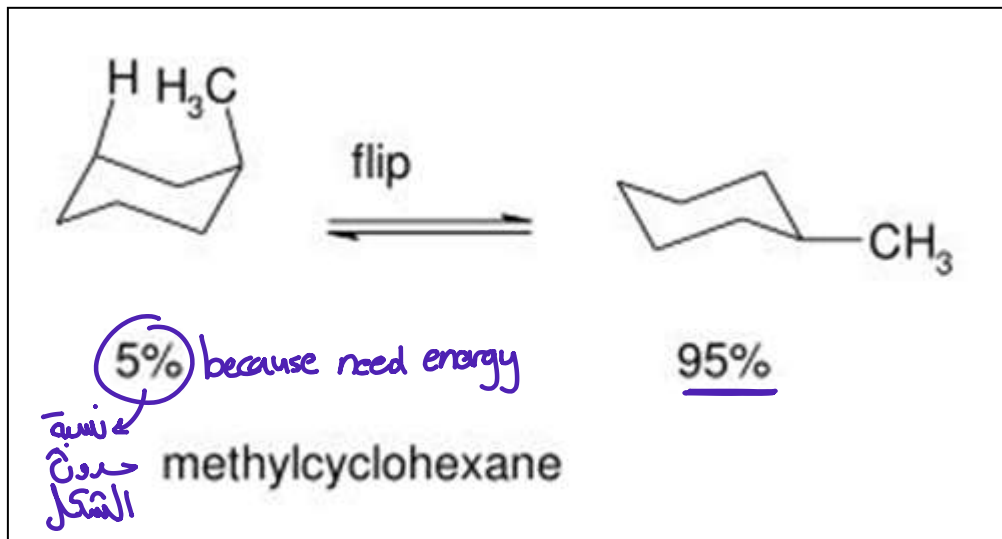


CH<sub>3</sub> in axial position  
position

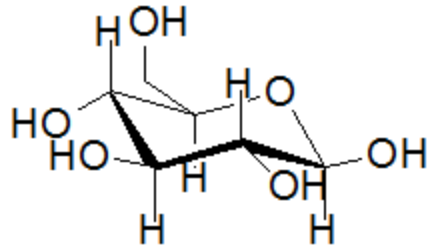


CH<sub>3</sub> in equatorial

is more stable



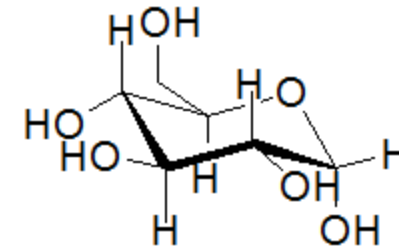
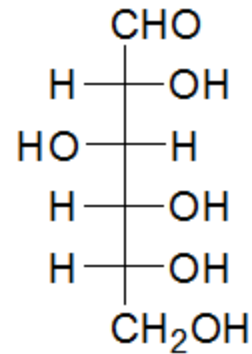
# Glucose molecule



beta-D-glucose

all OH groups equatorial

more stable



alpha-D-glucose

one group forced to be axial  
(equatorial 3W1)

ex: cyclopentane

(it can move)

name: half chair  
half boat  
(ألفا) envelope

