① AlKanes : Acyclic hydrocarbons which have a general formula [C_nH_{2n+2}]

* Each carbon is sp^3 hybridization (4 σ bonds).

* Physical properties :

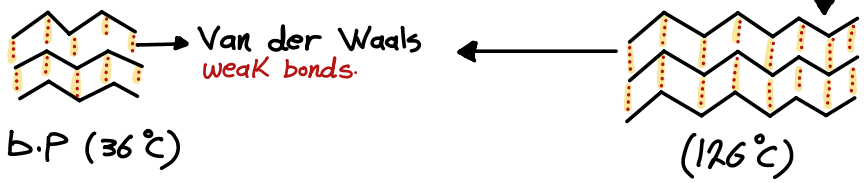
1 AlKanes are insoluble in H_2O due to the absence of hydrogen bonding with H_2O molecules. (hydrocarbones are [non-polar] molecule) ← C–H, C–C

* note : AlKanes are soluble in non-polar solvents.

2 Boiling points (BP) : In general alKanes have low b.P since inter-molecular force among alKane molecule is [Van der Waals]. → "weak forces"

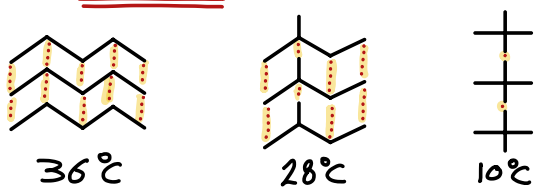
However, as molar masses of alKanes increases ⇒ b.p increases ↑

↳ increases in molecules →



b.P (36 °C) (126 °C)

* For identical molar masses, as symmetrical increases ⟶ b.P ↑



36 °C 28 °C 10 °C

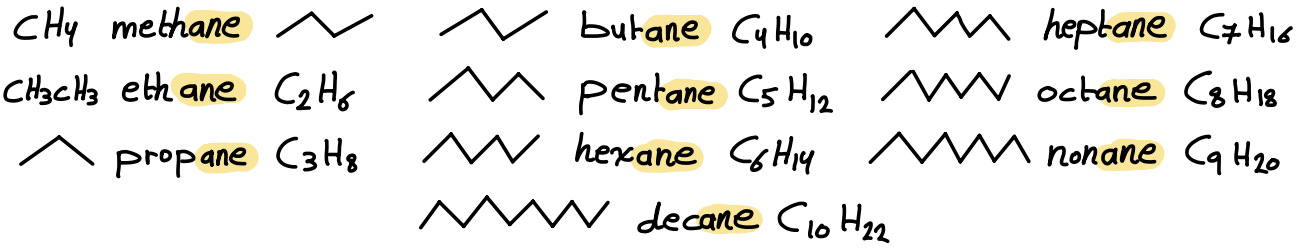
symmetrical ↑ symmetrical ↓

⟶ when two molecules have the same number of carbons, we must see the branches and which has less branches ⟶ high b.P.

* Nomenclature of AlKanes

⟶ IUPAC system and common names are used.

① IUPAC Rules :- [First] : for continous chain (unbranched alKanes).



✳ [second]: For branched alKanes

1] locate the longest continous carbon chain to determine the parent name.

2] Number the chain from the end nearer to the first substituent.

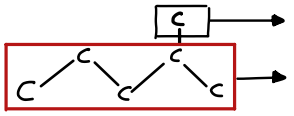
3] Determine the position of each substituent on the longest carbon chain.

4] If 2 or more identical substituents are present, use the prefixes di for 2, tri for 3, tetra for 4.

5] Write [substituents first] then parent name.

↳ based on alphabetical order.

Ex 1.



C → substituent

continous chain: parent name is pentane.

6] Naming of substituents:

Alkyl group $[C_nH_{2n+1}]$

- $-CH_3$: methyl
- $-C_2H_5$: ethyl
- $-C_3H_7$: } see the example
- $-C_4H_9$: }

Halogens

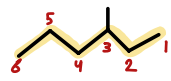
- F− : Fluoro
- Cl− : chloro
- Br− : Bromo
- I− : iodo

✳ $CH_3-CH_2-\tilde{C}H_2$ (propyl) $\quad CH_3-\tilde{C}H-CH_3$ (isopropyl) ⟶ About C_3H_7

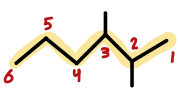
✳ $CH_3CH_2CH_2\tilde{C}H_2$ (butyl) $\quad CH_3\tilde{C}HCH_2CH_3$ (sec-butyl) } About C_4H_9

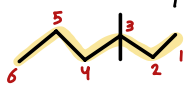
$H_3C(CH_3)CH-CH_2$ (isobutyl) $\quad CH_3-\overset{CH_3}{\overset{|}{\tilde{C}}}-CH_3$ (tert-butyl) }

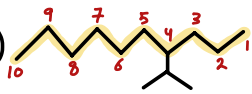
✳ Example of alKanes naming :-

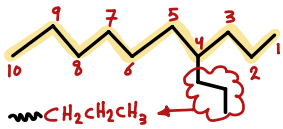
①  [3-methyl hexane]

position of sub — sub — parent

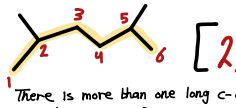
②  [2,3-dimethylhexane]

③  [3,3-dimethylhexane]

④  [4-isopropyl decane]

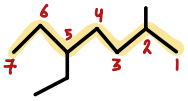
⑤ 

[4-propyldecane]

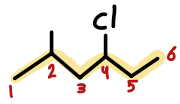
⑥  [2,5-dimethylhexane]

↳ There is more than one long c-chain but all are equal in number of substituent

⑦  [2,2-dimethylpropane]

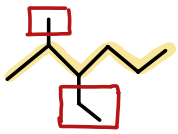
⑧  [5-ethyl-2-methylheptane]

↳ According to Alphabet

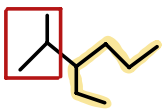
⑨  [4-chloro-2-methylhexane]

✳ Important notes :-

⑩ If you have 2 equal long of carbon chain, select one with the most branches.

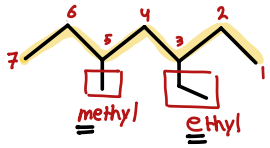


2-Substituents ✓



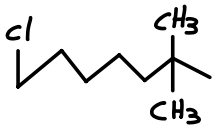
1- substituent X

⑪ If branching occurs at equidistent ⟶ number the chain from the end according to the alphabetical order of substituants.



From right → 3,5
left → 3,5
} equidistent
⇓ in this case
(alphabetical)

⑫ What is the correct numbering in the molecule ?



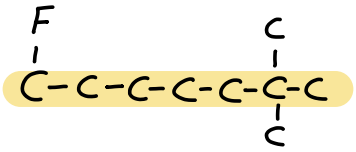
From right : 2,2,7 X
From left : 1,6,6 ✓

Just compare the first digit in each case (1<2) then select a lower one

Don't do a summation. How ?

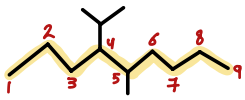
⑬ Prefixes : [di, tri, tetra, sec-, tert] are not included in Comparison of the alphabetical order of substituents But (iso) is included.

✳ Examples :-



1-Fluoro-6,6-dimethylheptane ✓

6,6-Dimethyl-1-fluoroheptane X

✳ 

4-Isopropyl-5-methylnonane ✓

5-methyl-4-isopropylnonane X

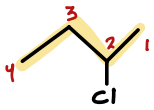
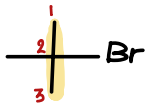
⑭ 

5-Bromo-2,2-dimethylhexane
not (2-Bromo-5,5-dimethylhexane)

From right → 2,2,5
left → 2,5,5
} we will choose the lower number

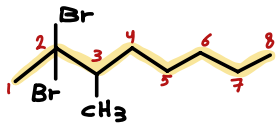
↳ No equidistant

✳ Common names : write organic part first

	IUPAC	Common
CH_3CH_2I	Iodoethane	Ethyl iodide
	2-Bromo propane	Isopropyl bromide
	2-chloro butane	sec-butyl chloride
	2-Bromo-2-methyl propane	tert-butyl bromide
CH_3F	Fluoromethane	methyl fluoride

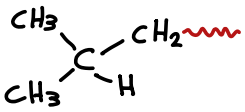
✳ Drawing of molecules :- start drawing of parent name , then number the chain from any end and finally , draw substituents.

a) 2,2-dibromo-3-methyl octane

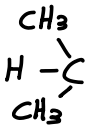


b) n-hexane

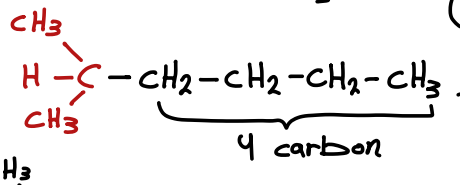
↳ normal (no branching)

c) Isobutyl 

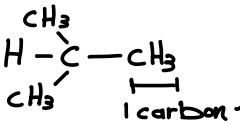
d) Propyl $CH_3CH_2CH_2$

e) Isoheptane : first draw (iso)  then draw 4-carbon atoms (7-3=4)

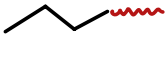
↳ common



→ 2-methyl hexane (IUPAC)

f) Isobutane :- 

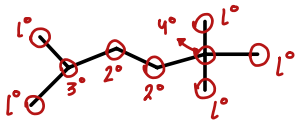
(4-3) = 1

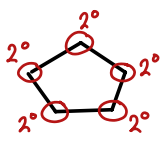
✳ butyl 

✳ Classification of carbon atoms :-

1° 2° 3° 4° ..... How ?

Primary secondary tertiary quaternary

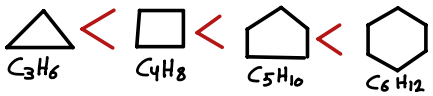




✳ note that the H-atom's classification is the same as the carbon it relates with.

✳ **CycloalKanes** : They are cyclic hydrocarbons with a general formula C_nH_{2n}

→ Examples :



The most stable (the least strained)

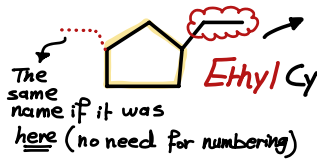
The least stable (the most strained)

→ far away from the Sp^3 angle

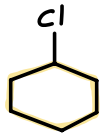
→ The actual angle is 109.5° like in Sp^3 (109.5°). (most stable)

✳ Naming of CycloalKanes :-

① Presence of (1) substituent (no need for numbering)

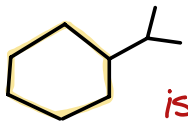


Ethyl Cyclopentane



chloro cyclohexane

methyl cyclopropane

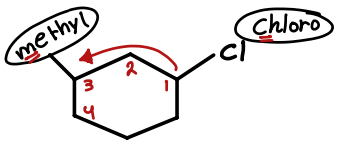


isopropyl cyclohexane

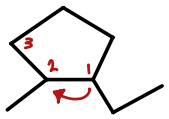
② Presence of (2) substituents

a) Give no (1) for carbon (in the Cyclic) that has a substituent based on alphabetical order.

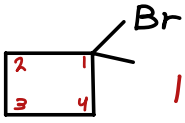
b) Give the second substituents a lower number.



1-chloro-3-methyl Cyclohexane



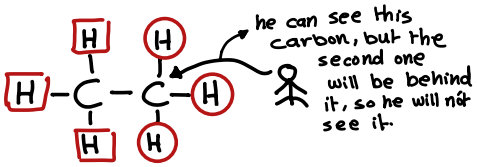
1-Ethyl-2-methyl Cyclopentane



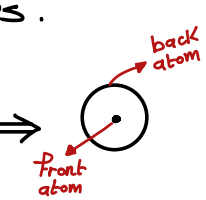
1-Bromo-1-methyl Cyclobutane

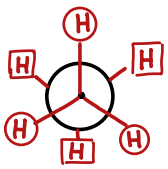
✳ Conformation of alKanes and CycloalKanes.

→ First : AlKane

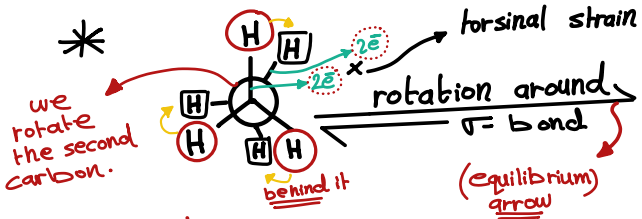


[Ethane]

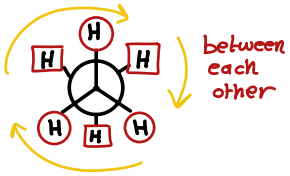




Newman projection



eclipsed conformer (less stable)



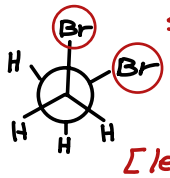
staggered conformer (more stable)

* The relationship between these two structures is conformer or (conformational isomers)

* Conformers (conformational isomers) :- They are isomers (same molecular formula) with same arrangments of atoms (not constitutional isomers) ; they are obtained by [interconvertible rotation] around σ-bond (single bond).

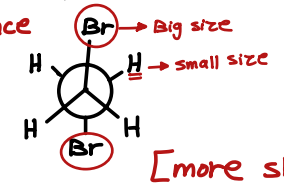
⟶ Eclipsed conformers are less stable than staggered since there is a torsinal strain in the eclipsed.

* Example 2 :- Draw the most stable conformer of 1,2-Dibromo ethane (CH_2Br-CH_2Br) ⇛



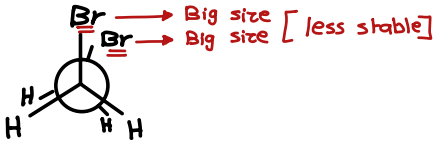
[less stable]

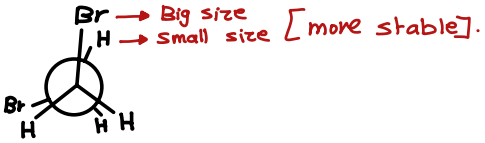
or



[more stable]

* Example 3 :- Draw the least stable conformer.

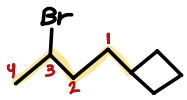




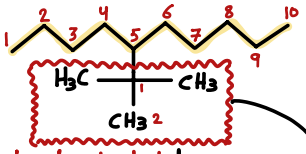
* General Examples :-

① 

3-Cyclopropylhexane

② 

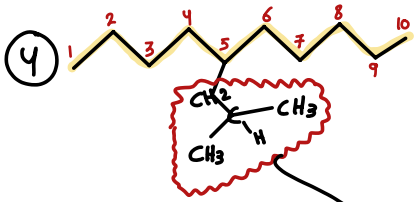
3-Bromo-1-Cyclobutylbutane

③ 

5-tert-butyldecane

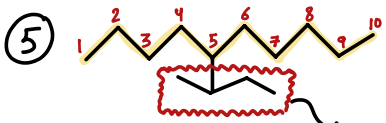
* we can name it by :

A) tert-butyl B) 1,1-dimethyl ethyl

④ 

5-Isobutyldecane

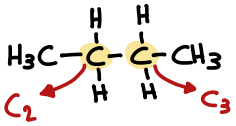
Isobutyl (2-methylpropyl)

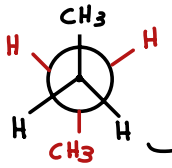
⑤ 

5-sec-butyldecane

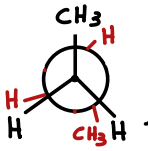
sec-butyl (1-methylpropyl)

✳ example about conformers :- Try butane →





(staggered)

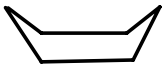


(eclipsed)

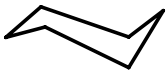
✳ Conformation of Cyclohexane : It has no angle strain (bond angle 109.5°).

→ Two conformational structures are present :

The most stable (no angle strain)



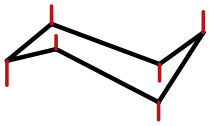
boat (less stable)



chair (more stable)

} → { conformational } isomers

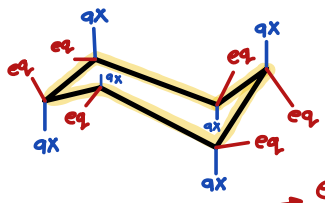
↳ In chair conformation , each carbon has 1 axial bond (⊥ on the plane)



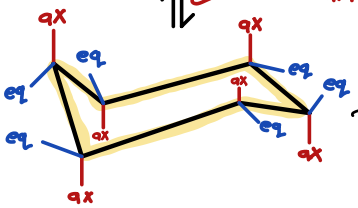
↳ and 1 equatorial bond (in the plane)

✳ If ring flips ⇒ each (ax) bond becomes (equatorial) bond and each (eq.) bond becomes an (ax.) bond.

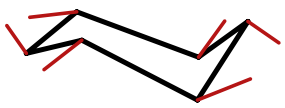
✳ Examples :-

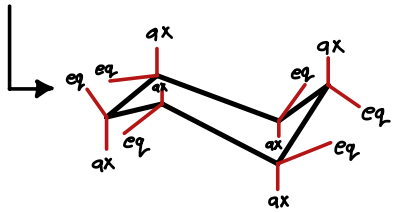


equilibrium arrow



[Conformational isomers]

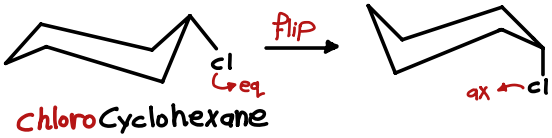




notes that the blue axial bond in the first structure flips so it becomes blue eq bond in the second structure , and this As well happens in red eq bond.

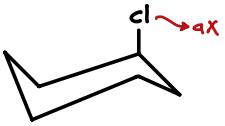
✳ Do a ring flip for :-

a)



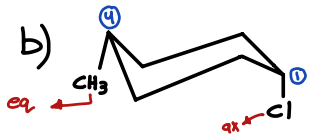
Chlorocyclohexane

or

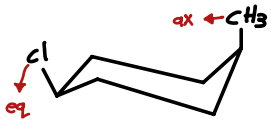


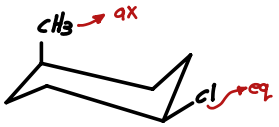
✳ note : you can choose any carbon to put the Cl on.

b)



Flip →

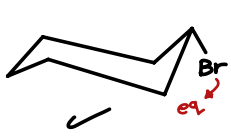




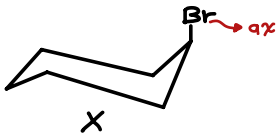
1-chloro-4-methyl Cyclohexane

* It doesn't matter which carbons you choose as long as the relationship between the two carbons is (1-4).

* Draw the most stable chair conformation of Bromo Cyclohexane.



✓

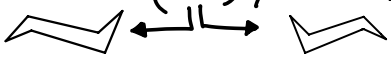


X

* notes: eq is more stable than ax.

→ Doesn't matter which carbon you choose.

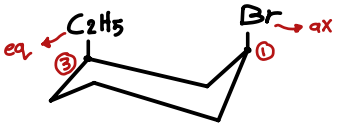
→ Doesn't matter which (chair) you choose.



* Equatorial bond is more stable than an axial bond and large groups (atoms) prefer (eq).

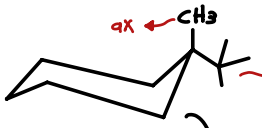
[↓ in periodic table, the size ↑]

* Draw the least stable chair conformation of 1-Bromo-3-ethyl Cyclohexane.



* you can select any chair structure any two carbons (1-3).

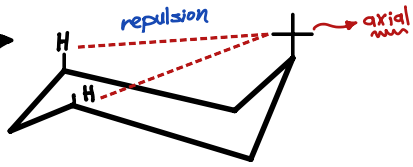
* Draw the most stable chair conformation of 1-tert-butyl-1-methyl Cyclohexane



(because tert-butyl is larger than methyl so tert-butyl prefer to be (eq) → more stable.

→ if you need the least stable just make the methyl (eq)

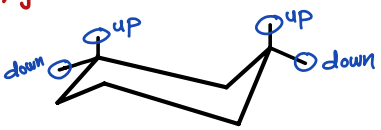
* The reason about why large groups prefer to be (eq) and its more stable is (1,3-Diaxial repulsion) and this doesn't happen in equtorial bonds.



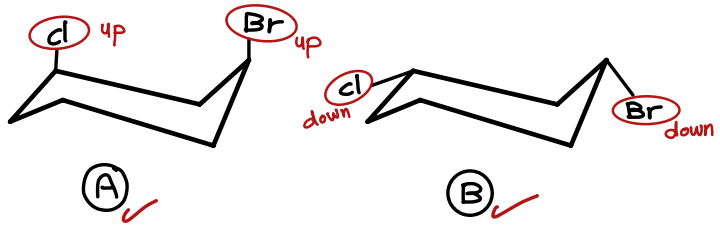
* Finally, cis-trans concept

No relation between (up, down) and (eq, ax).

2 substituents are up, up → or down, down → } cis while up, down → } trans

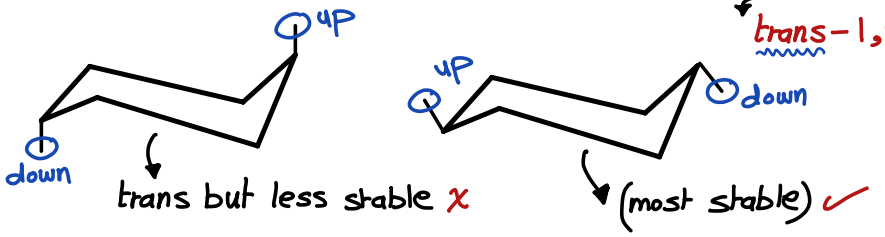


✳ Example 1 :- Draw Cis-1-Bromo-3-chloroCyclohexane in chair conformation

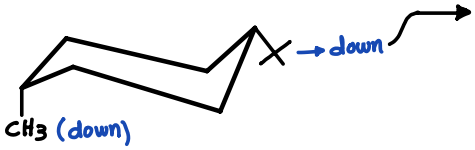


✳ Both structures A+B is true (but) if we were asked about stability B is more stable (eq).

✳ Example 2 :- Draw the most stable conformer of trans-1,4-dimethyl Cyclohexane



✳ Example 3 :- Draw the most stable conformer of Cis-1-tert-butyl-4-methyl Cyclohexane



remember that large group (tert-butyl) prefer to be eq to be more stable.

✳ Cis-trans isomerism in CycloalKanes.

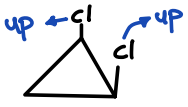
✳① If a Cyclic has 2 substituents (not 1 or 3) and these 2 substituents are not located at Same carbon. ⇒ we should use the term of Cis-trans.

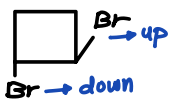
✳② Cis : Same side (up-up) or (down-down).

trans : opposite side (up-down).

✳③ Include cis-trans in the naming of the molecule.

✳④ Assign the following as cis, trans or none.

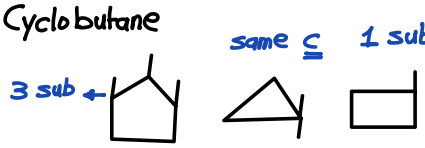




Cis-1,2-dichloro Cyclopropane

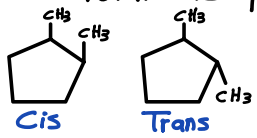
trans-1,2-diBromo Cyclobutane

trans-1-chloro-3-methyl CyclePentane



no (trans-cis)

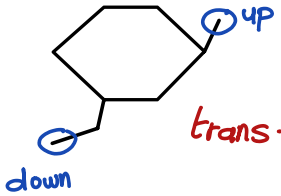
✱⑤ The relationship between :-



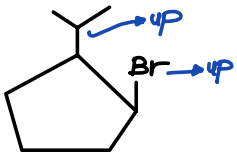
✱ cis-trans isomerism "geometric isomers" → These isomers can't be generated by rotation around σ-bond.

✱⑥ They have different physical properties (boiling points, melting points) and can be separated using physical methods (such as distillation).

✱⑦ Name the following molecules :-

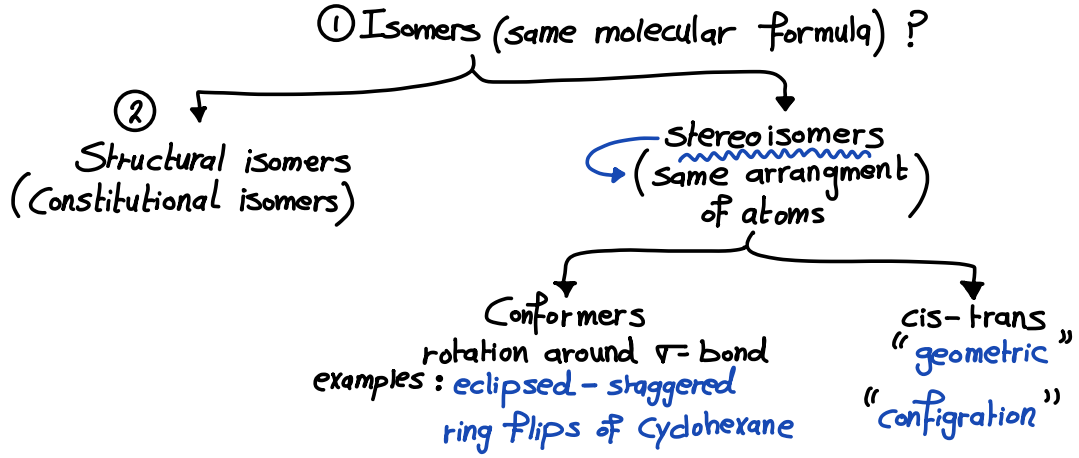


trans-1-ethyl-3-methyl Cyclohexane

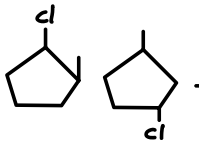


Cis-1-Bromo-2-isopropyl Cyclopentane

✱ Summary of Isomerism :-



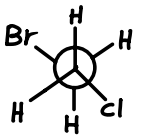
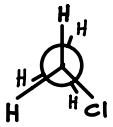
✱ Note :- You can't find a relationship between (cis-trans) and (conformers) at the same time.

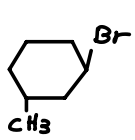
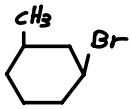
① 

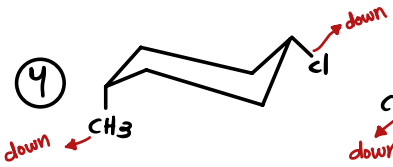
→ Are they isomers ? yes (have the molecular formula)

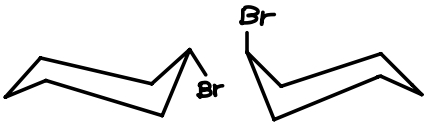
Are they have the same arrangment of atoms ? no

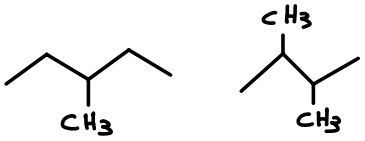
→ structural isomers (constitutional)

②   → Are they isomers? no.

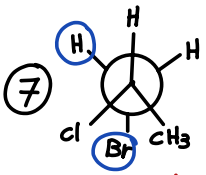
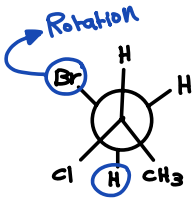
③   → cis-trans isomers (geometric)

④  → conformers "ring flips".

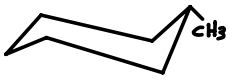
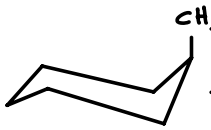
⑤  → conformers "ring flips".

⑥  → constitutional isomers.

C_6H_{14} C_6H_{14}

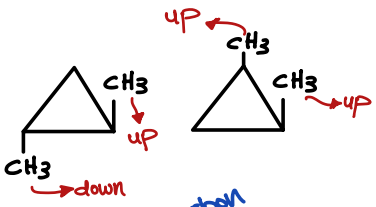
⑦   → conformers.

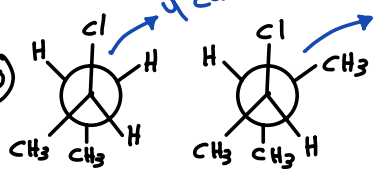
staggered staggered

⑧   → the same arrangment of atoms.

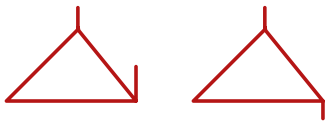
not [cis-trans] because there is 1 sub.

methylCyclohexane methylCyclohexane → conformers [even if the chair isn't inverted we can say that this is ring flip]

⑨  → cis-trans.

⑩  → not isomers (different molecular formula).

* Example :- Draw C_5H_{10} that can show cis-trans isomerism.



cis trans

* Example :- Draw C_5H_{10} that contains only secondary carbons.

* Reactions of Alkanes.

① Combustion of hydrocarbons → alkane, alkene, alkyne

$$CH \xrightarrow[\text{spark}]{O_2} CO_2 + H_2O + \text{heat}$$

"exothermic".

② Radical substitution reaction.

↳ odd number of electrons ; it is very reactive.

examples :- $:\dot{\underset{\cdot\cdot}{\underset{\cdot\cdot}{Cl}}}\cdot$, $:\dot{\underset{\cdot\cdot}{\underset{\cdot\cdot}{Br}}}\cdot$, $\dot{C}H_3$

$$CH_4 + Cl_2 \xrightarrow{\Delta \text{ or } h\nu} CH_3Cl + HCl$$

monochlorination

$$CH_3CH_3 + Br_2 \xrightarrow{h\nu} CH_3CH_2Br + HBr$$

$BrCH_2CH_3$ is also possible

monobromination

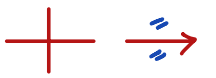
* How many products whould you prepared upon monobromination of :-

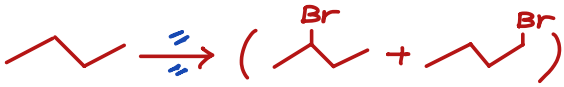
$CH_4 \xrightarrow[h\nu]{Br_2}$ 1 (CH_3Br).

$CH_3-CH_3 \rightrightarrows$ 1 (CH_3CH_2Br).

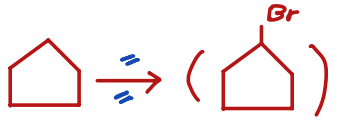
 $\rightrightarrows$ 2 ($CH_3CH_2CH_2Br$ + $CH_3\underset{\displaystyle Br}{\underset{|}{C}}HCH_3$)

constitutional isomers


(1 product).



2 products.

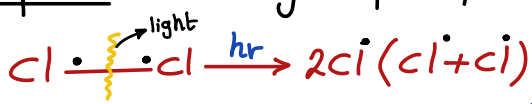


1 product

✳ Different environment of H will produce different products (structural isomers).

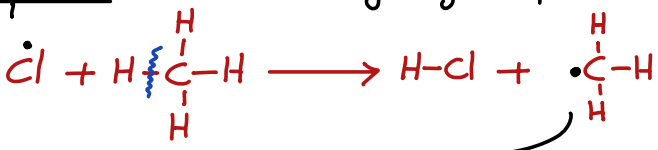
✳ Mechanism of reaction :-

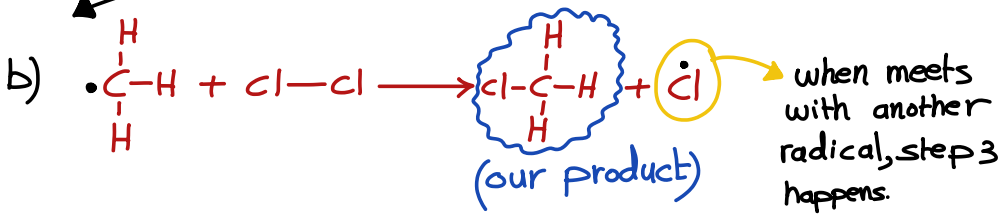
step 1: Initiating step : Production of radical.



low amount of Cl_2 is consumed.

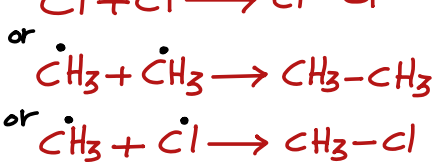
step 2: chain-Propagating step:-

a) 

b) 

✳ Radical is consumed in reactant and another radical is produced in product. step 2 will be repeated to get more.

step 3 : chain- Terminating step



✳ Radical is consumed and no radical is produced.

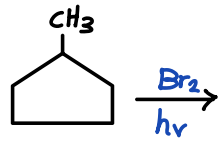
* General Notes Regarding chapter 2 :-

① Radical Substitution Reaction

$CH_4 + Cl_2 \xrightarrow{\text{(excess)}} CH_3Cl \hookrightarrow CH_2Cl_2 \hookrightarrow CHCl_3 \hookrightarrow CCl_4$ } this consider disadvantage.

Mixture of products is obtained.

* How many products could be obtained upon monobromination reaction of.

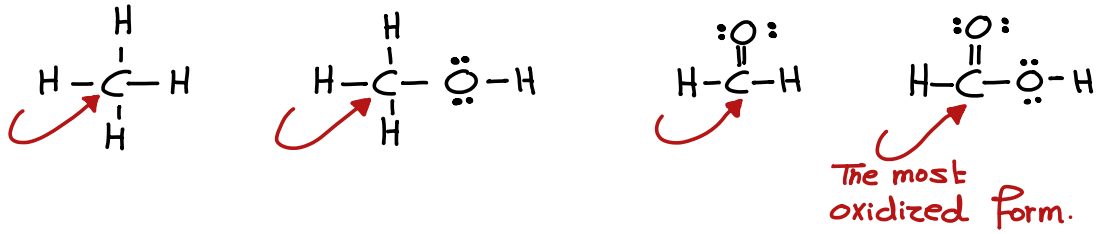


* Draw an alkane that may produced in the termination step for the reaction :-

$CH_3CH_3 \xrightarrow[hv]{Br_2} CH_3CH_2Br + HBr$

→ answer :- butane

② In Combustion Reaction



③ Et- stands for CH_3CH_2- , Me- stands for CH_3- , i-Pr- stands for CH_3CHCH_3

The End of chapter 2

Done by : Sultan Ghaith