chapter (1) : Bonding and Isomarism.

mass number ← A, atomic number ← Z, $^{A}_{Z}X$

1] Electron configuration of an atom.

$^{12}_{6}C \rightarrow 1s^2 2s^2 2p^2$ → valence electrons. $^{16}_{8}O \rightarrow 1s^2 2s^2 2p^4$ → valence electrons.

The $\bar{e}$ that involve formation of bonds

atomic orbitals

* valence electrons : electrons that locate in the most outer shell [the highest value of n] * note : valence electron of an atom = number of group of atom.

* valency of an atom [8 - group number] → ex : valency of oxygen = 2.

2] Ionic and covalent bonds → 95% of organic compound is covalent.

cation (+)	anion (-)
- metals (Li, Na, K)	- non-metals (H, C, N, O, halogens)
- lose $\bar{e}$.	- gain $\bar{e}$.

* Examples of Ionic compounds [metal + non-metal]

$NaOCH_3$: Na^+ cation, OCH_3^- anion

KCN : K^+ cation, CN^- anion

$LiSCH_3$: Li^+ cation, SCH_3^- anion

* Example of covalent molecules : [All the atoms are non-metal]

H_2O (non-metal, non-metal) Cl_2 (non-metal) CH_4 (non-metal, non-metal)

* Bond energy : energy required to breaK 1 mol of bond (endothermic).

weakest ← C-C < C=C < C≡C → strongest

* Bond length : distance between two nuclei of atoms.

* As Bond energy ↑, the bond length ↓.

Exercise : which atom is more electronegative ? { electronegativity increase from → ↑ }

N or F ? F F or I ? F

→ which atom is more electropositive ? { electropositivity increases from ↓ ← }

Li or Be ? Li Li or Na ? Na

* Covalent bond could be :-

- Non-polar: H-H (non-metal, non-metal), Cl-Cl, Br-Br, C-H → The difference is so small.
- Polar: C-O, C-N, C-F, C-Cl, H-O, H-N

* Polar covalent bond means : Partial charges (δ) is present, such as

$C^{\delta+}-F^{\delta-}$

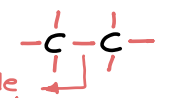
$C^{\delta+}=O^{\delta-}$ → oxygen is more electronegativity than C.

→ Define electronegativity : Ability of an atom to withdrawn electrons (in the bond) to itself.

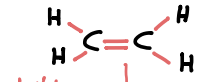
* Exercise : which bond is the most polar ?

identical ← C-O (A) C-F (B) C-N (C) C-Cl (D)

✳ Define : hydrocarbons :- compounds contain only carbons and hydrogen atoms.

→ They could be :  (⟷) ← σ

single bond ← σ



double bond and which has σ and π

↳ Triple bond and which has a σ and 2π

↳ side by side

✳ note : σ bond is stronger than (π) bond.

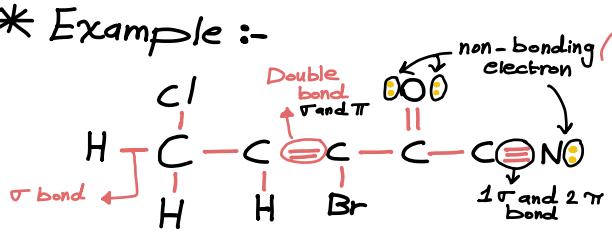
→ Remember : Carbon atom can form maximum (4 bonds) and hydrogen (one) bond.

✳ Alkanes : no double bonds nor triple bonds.

✳ Alkenes : contain carbon-carbon double bond (C=C).

✳ Alkynes : contain carbon-carbon triple bond (C≡C).

✳ Example :-



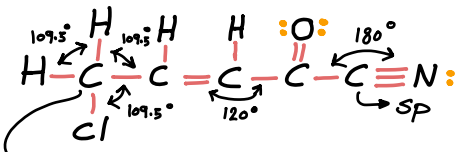
✳ σ bond head by head overlap while π bond is side by side.

✳ C-N : < C=N : < C≡N : → The strongest and shortest bond.

✳ Hybridization of Carbon atom.

→ It could be [sp . sp^2 or sp^3].

✳ example :-



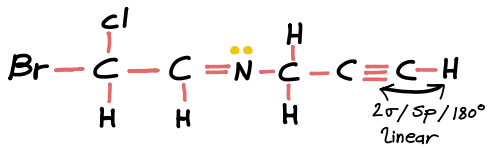
✳ If carbon atom forms 4σ bonds ⇒ hybridization is : sp^3 bond angle 109.5° and geometry is Tetrahedra (Td).

✳ If carbon atom has 3σ bonds ↩ sp^2, 120°, trigonal planar.

✳ If carbon atom has 2σ bonds ↩ sp, 180°, linear.

→ note : when you were asked about angle look at the center.

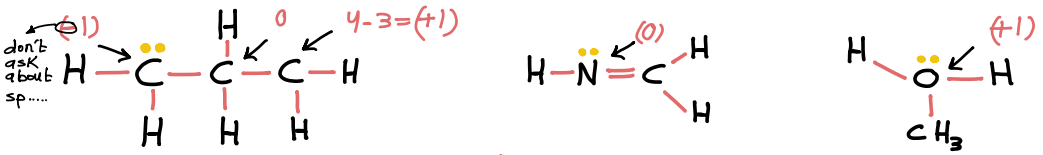
✳ Exercise :



✳ Resonance structures : when you draw a resonance structure, σ-bond and atoms are localized, while π-bonds (π-electrons) and lone pair of electrons are delocalized.

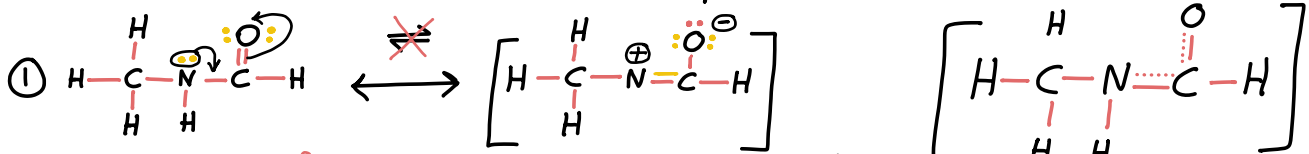
✳ Formal charge of an atom : actual change of a given atom.

→ Examples : Calculate the formal charge for indicated atoms, Knowing that the atomic number of C : 6 , N : 7 , O : 8



✳ Formal charge = [number of valence e⁻ in an isolated atom (group number)] − [number of intervening e⁻ around atom after homolytic cleavage ↳ breakdown]

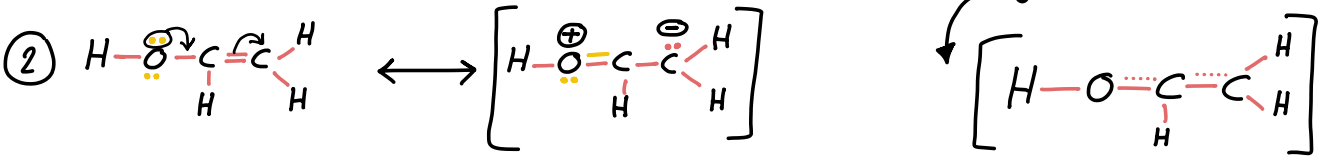
✳ Draw a resonanse structure and hybrid structure for :-

① 

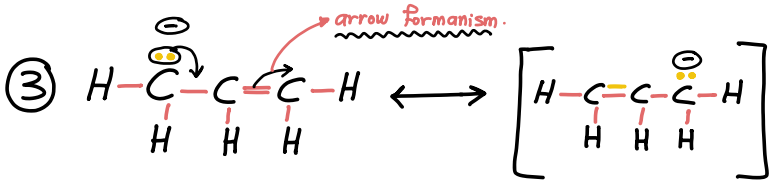
✳ note that (N) can form 3 bonds.

(II) second resonanse structure

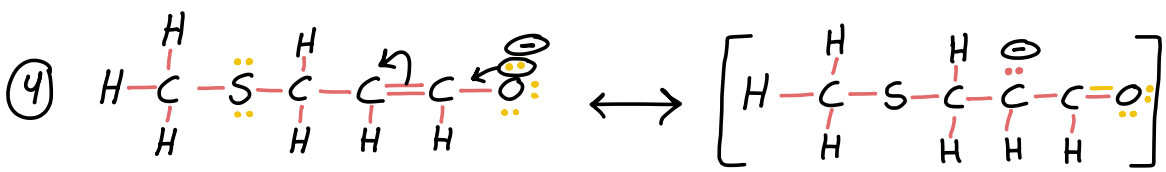
hybrid structure

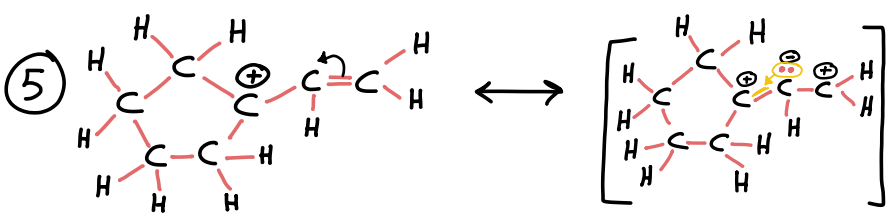
② 

(II) second resonanse structure

③ 

✳ (·····) → stronger than single bond and weaker than double bond.

④ 

⑤ 

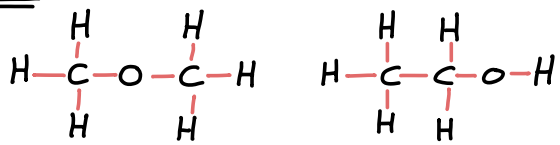
✳ There is more stable resonanse will less formal charges → (−).

✳ when a carbon atom in a Hybridization of a sp^3 don't touch it. ← important notes

✳ Total formal charges is equal in both structures.

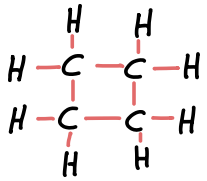
✳ Isomers : molecules have the same molecular formula. ⟶ Bond dosent matter.

example :-

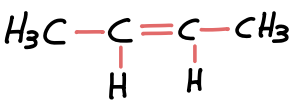


$[C_2H_6O]$ $[C_2H_6O]$

example 2 :-



$[C_4H_8]$



$[C_4H_8]$

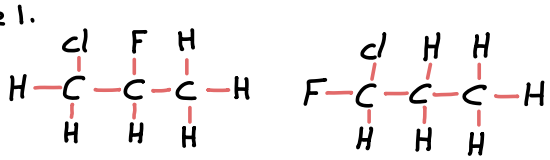
⟶ Ary they isomers ? yes.

⟶ Are they isomers ? yes.

⟶ Two molecule is considered isomers if they are identical.

✳ Define constitutional isomers (structural isomers) ? have same molecular formula but different arrangement of atoms.

⟶ example 1.



(A) (B)

⟶ Are they constitutional isomers ?

step 1 Are they isomers ?

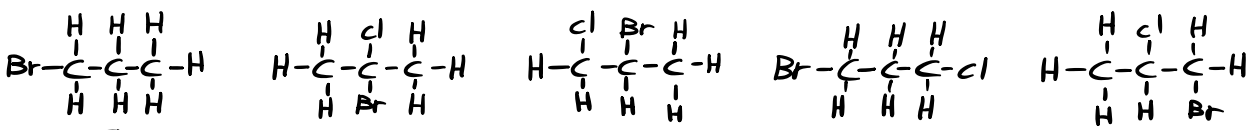
A: C_3H_6ClF B: C_3H_6ClF

[identical] so yes.

step 2 Have they different arrangement of atoms ? yes

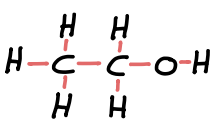
✳ Isomers → Constitional isomers (structural isomers).
→ ???....?

✳ Draw (5) constitutional isomers of C_3H_6BrCl ?



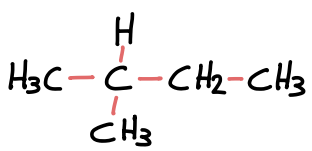
① ② ③ ④

⟶ Abbreviated structural formulas :

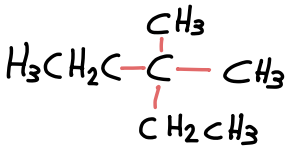
①  ≡ CH_3-CH_2-OH (CH_3CH_2OH).

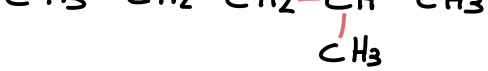
② $CH_3-CH_2-CH_2-CH_2-CH_3$ ≡ $CH_3-(CH_2)_3-CH_3$

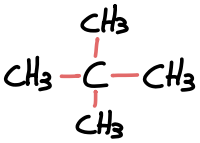
✳ Expand the following formula :-

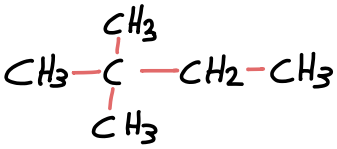
① $(CH_3)_2CHCH_2CH_3$ ⟶ 

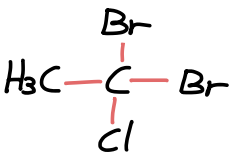
Don't start with (−).

② $(CH_3CH_2)_2C(CH_3)_2 \longrightarrow$ 

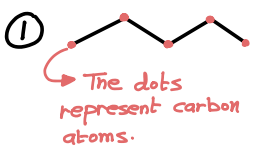
③ $CH_3(CH_2)_2CH(CH_3)_2 \longrightarrow$ 

④ $(CH_3)_4C \longrightarrow$ 

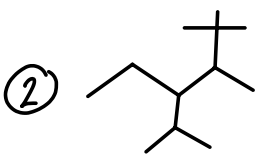
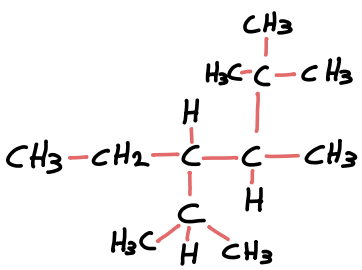
⑤ $CH_3C(CH_3)_2CH_2CH_3 \longrightarrow$ 

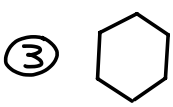
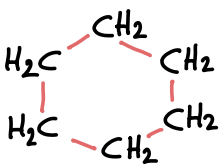
⑥ $CH_3CBr_2Cl \longrightarrow$ 

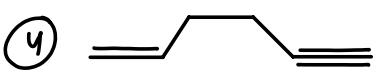
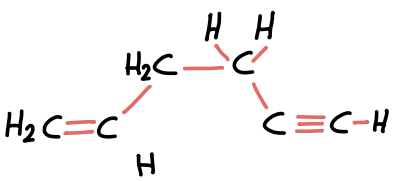
✱ Line bond formula : (important)

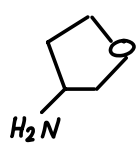
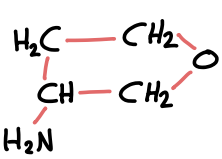
① 

$\longrightarrow CH_3-CH_2-CH_2-CH_2-CH_3$

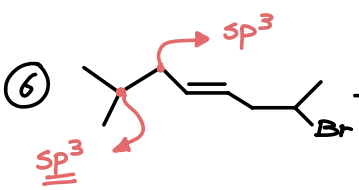
②  $\longrightarrow$ 

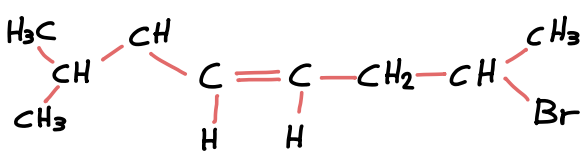
③  $\longrightarrow$ 

④  $\longrightarrow$ 

⑤  $\longrightarrow$ 

✱ remember : each carbon has H bonds.

⑥ 

$\longrightarrow$ 

✱ You might be asked about molecular formula in each above example.

✱ Functional group : certain arrangment of atoms.

1] Only C–C and C–H $\longrightarrow$ alKanes.

2] C=C $\longrightarrow$ alKene 3] C≡C $\longrightarrow$ alKyne

4]  ⟶ Arene "Aromatic" (3 double bond.)

5] C–X ⟶ alkyl halide (halogens)

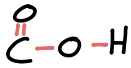
6] C–OH ⟶ Alcohol

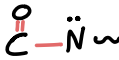
7] C–O–C ⟶ ether

8]  ⟶ Aldehyde

9]  ⟶ Ketone

10]  ⟶ ester

11]  ⟶ Carboxyle acid

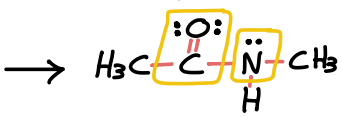
12]  ⟶ Amide

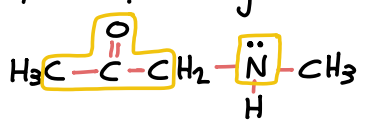
13]  ⟶ Amine

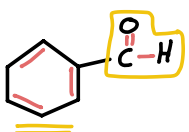
14] C–S–C ⟶ sulfide

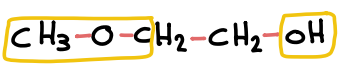
⟶ Now, go to specific examples :-

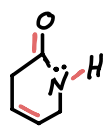
✳ Find functional groups in each of the following structures ?

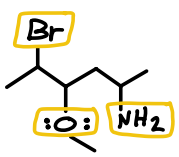
⟶  (Amide)

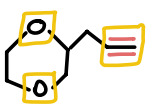
⟶  (Ketone + amine)

⟶  (Aromatic + Aldehyde)

⟶ 
(ether + alcohol)

⟶  (Amide + alkene)

⟶  (Alkyl halide + ether + Amine)

⟶  (ether (2) + Alkyne)

⟶  (Alkene)

✳ Also, in each molecule, write :

1] molecular formula

2] hybridization for each atom.

3] Bond angle for each

4] Geometry for each carbon

5] Number of carbon – carbon double bond

✳ note : when question ask you about formal charge (don't complete) the hydrogen.

The End of chapter 1

Done by : Sultan Ghaith