Chapter 1. Bonding and Isomerism

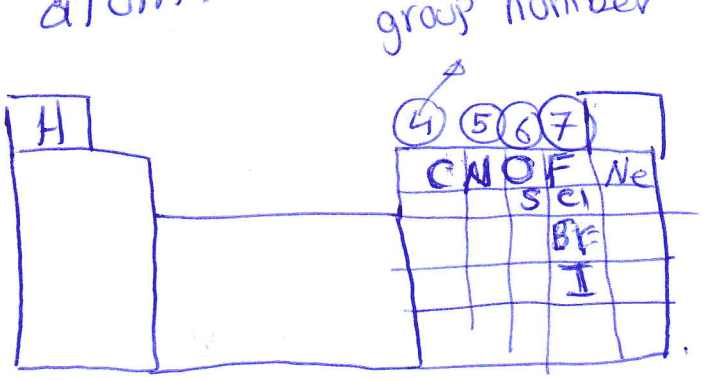
① Electronic configuration of an atom

$^{12}_{6}C$ $1s^2 2s^2 2p^2$ Valence electrons: 4

$^{1}_{1}H$ $1s^1$ " : 1

$^{16}_{8}O$ $1s^2 2s^2 2p^4$ " : 6

* Valence electrons: electrons that locate in the most outer shell. (the highest value of n).
* Valence electrons of an atom equals group number of that atom.



Valency of Oxygen = 2, Valency of Cl = 1

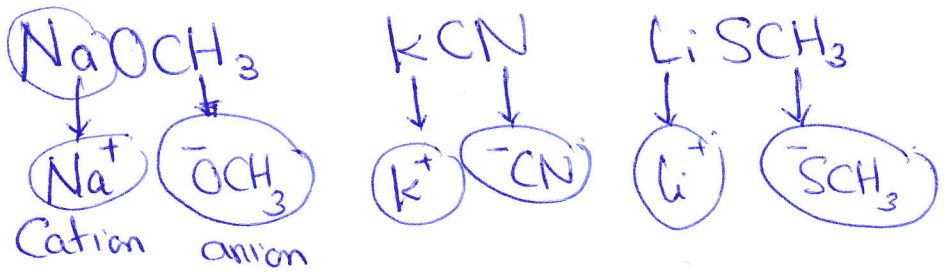
" " Carbon = 4

② Ionic and covalent bonds.

Metals (Li, Na, k) → lose electrons

Non-metals (H, C, N, O, halogens) → gain electrons.

* Examples of Ionic Compounds: Metal with Non-metal



* Examples of covalent molecules:- All atoms are non-metals.

H_2O Cl_2 H_2 CH_4

* Bond energy: energy required to break 1 mol of bond (Endothermic)

$C-C < C=C < C\equiv C$

* Bond length: distance between two nuclei of atoms.

As Bond energy ↑, the bond length ↓.

Exercise: Which atom is more electropositive?

Li or Be ?

Li or Na ?

Exercise: Which atom is more electronegative?

N or F ?

F or I ?

* Covalent bond could be :-

Non-Polar

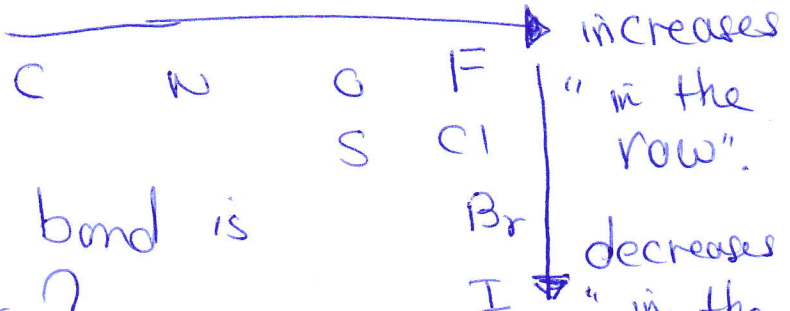
H – H
Cl – Cl
Br – Br
C – H

Polar

C – O
C – N
C – F
C – Cl
H – O
H – N

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

* Define electronegativity :- Ability of an atom to withdrawn electrons (in the bond) to itself.

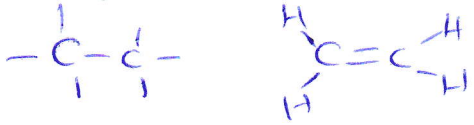


* Exercise :- which bond is the most polar ?

C – O (A) C – F (B) C – N (C) C – Cl (D)

* Define hydrocarbons :- Compounds contain only carbon and hydrogen atoms.

They could be :-



H – C ≡ C – H

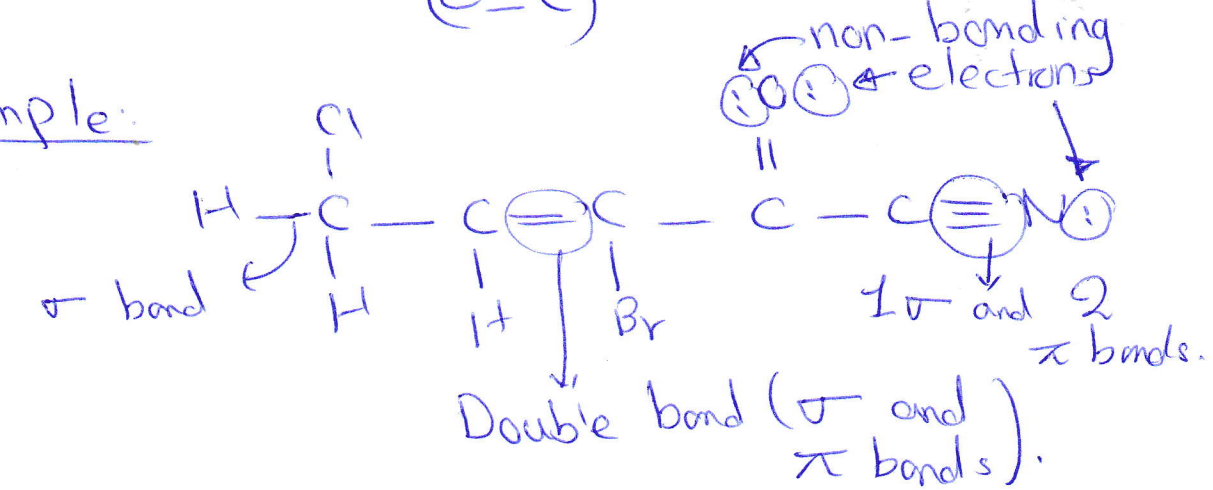
Remember: * Carbon atom can form maximum 4 bonds and hydrogen atom one bond.

* alkanes:- no double bonds nor triple bonds.

alkenes:- Contain carbon-carbon double bond (C=C)

alkynes:- Contain carbon-carbon triple bond (C≡C)

Example:



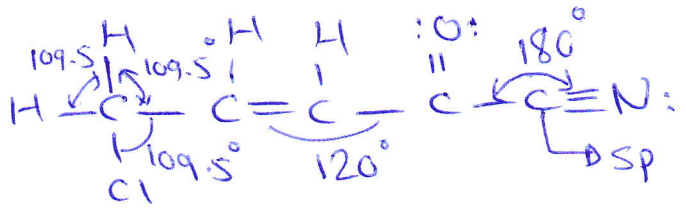
σ-bond: head by head overlap, while π-bond is side by side overlap. σ-bond is stronger than π-bond.

C-N: < C=N: < C≡N: the strongest bond

C-C < C=C < C≡C

* Hybridization of Carbon atom

It could be sp, sp^2 or sp^3.

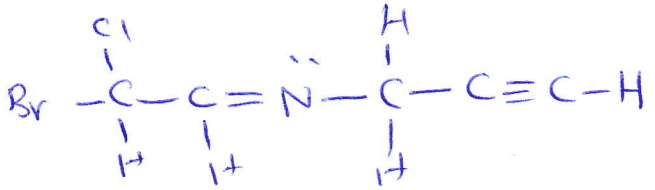


If Carbon atom forms 4 σ bonds ⟹ hybridization is: sp^3, bond angle 109.5° and geometry is Tetrahedral (T_d).

If C-atom has 3 σ bonds ⟹ sp^2, 120°, trigonal planar.

If C-atom has 2 σ bonds ⟹ sp, 180°, linear

Exercise:

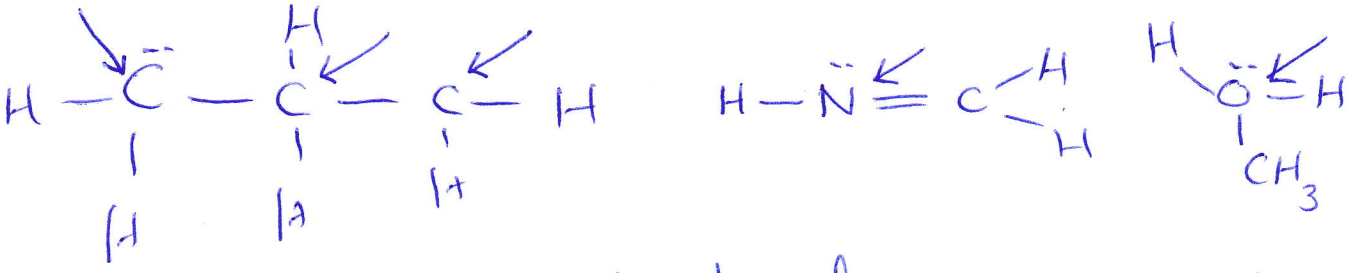


Find, hybridization, bond angle and geometry of each.

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

* Formal charge of an atom:- actual charge of a given atom.

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

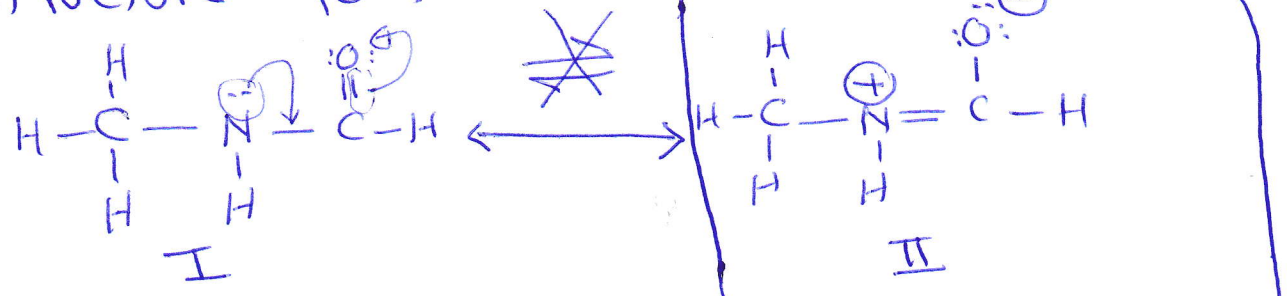


Formal charge = (number of valence electrons in an isolated atom) − (number of intervening electrons around atom after homolytic cleavage)

(−1) (zero) (+1) (zero) (+1)

Draw a resonance structure and hybrid structure for:-

(1)

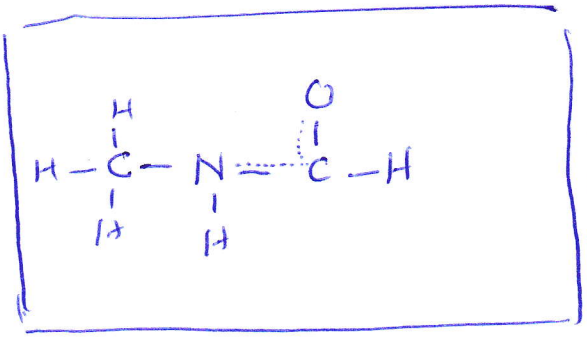


I

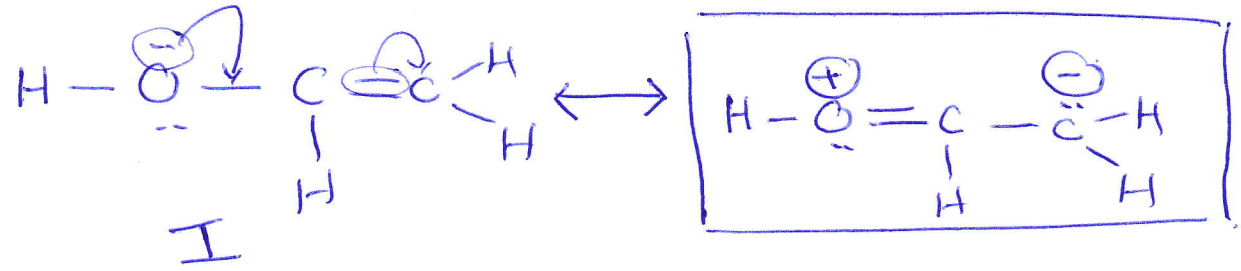
II

second resonance structure

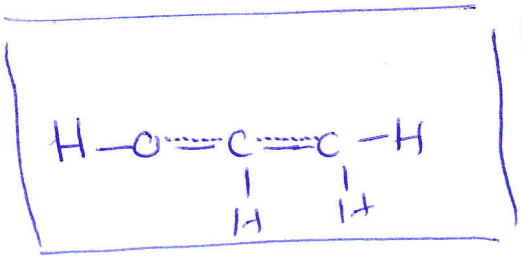
* Total formal charges are equal on both structures.



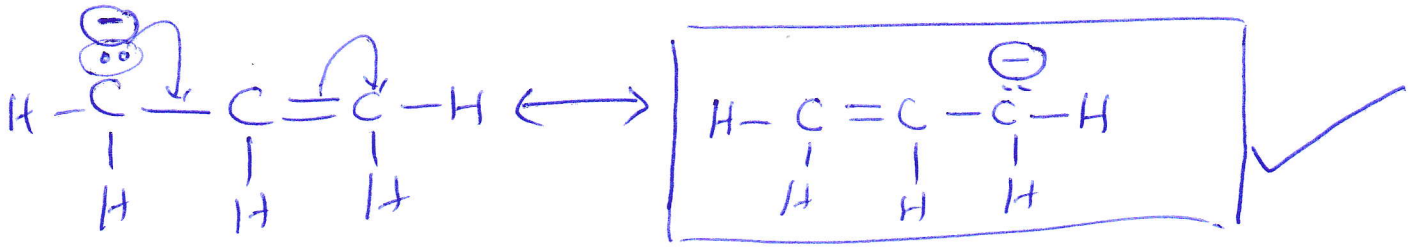
hybrid structure: real structure

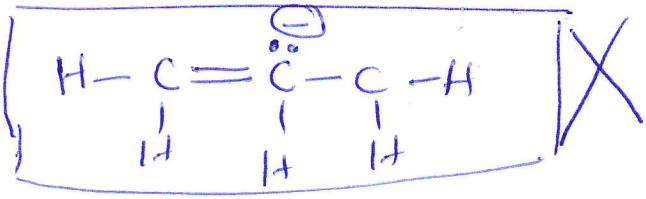
② 

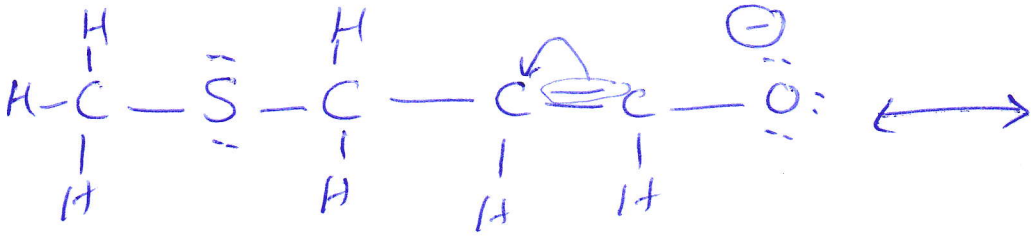
I

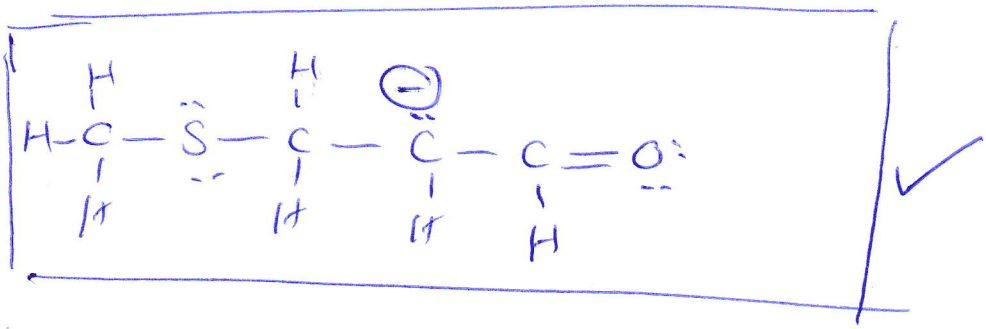


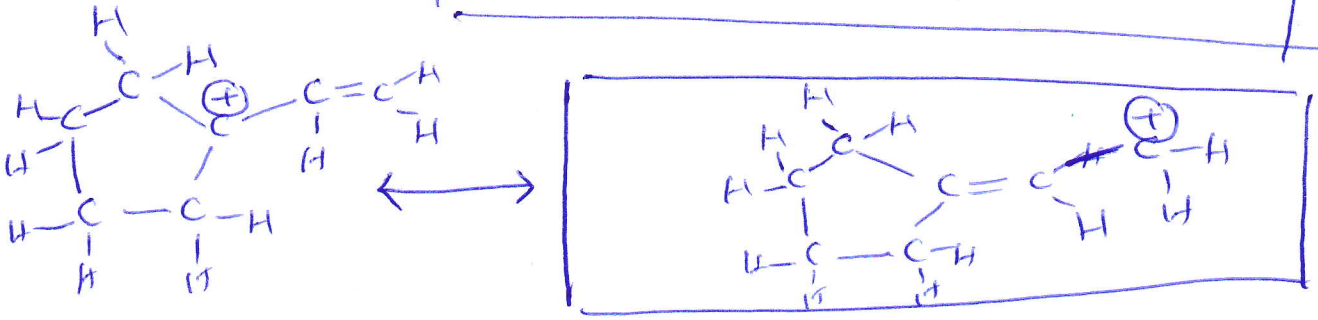
hybrid structure

③ 



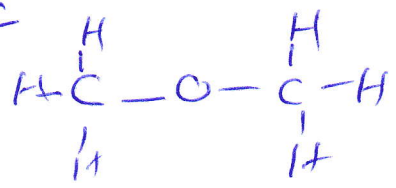
④ 



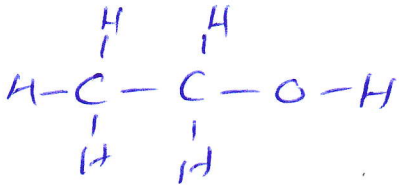
⑤ 

Isomers: Molecules have the same molecular formula.

Ex1.



C_2H_6O

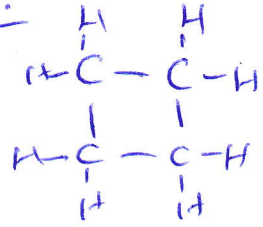


C_2H_6O

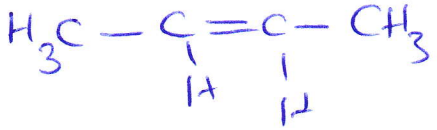
Are they isomers?

Yes

Ex2.



C_4H_8

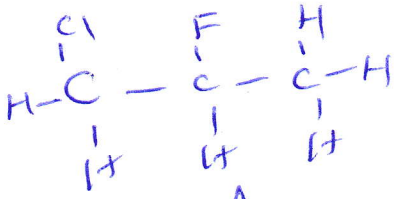


C_4H_8

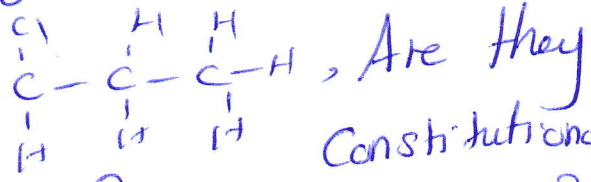
Yes

Define Constitutional isomers (structural isomers)? have same molecular formula but different arrangment of atoms.

Ex1.



A



B

Are they Constitutional isomers?

Step 1: Are they isomers? A: C_3H_6ClF B: C_3H_6ClF

Yes.

Step 2: Have they different arrangment of atoms?

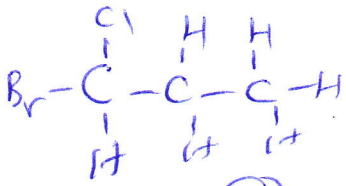
Yes.

So, they are Constitutional isomers.

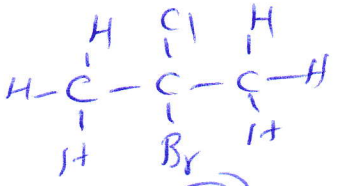
Isomers

- Constitutional isomers (structural isomers).
- ???

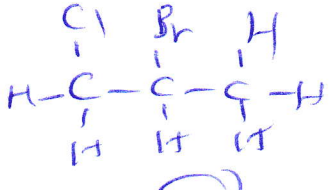
* Draw 5 Constitutional isomers of C_3H_6BrCl?



(1)



(2)



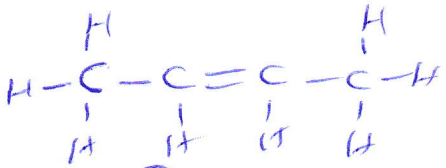
(3)

(4)

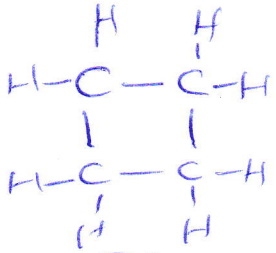
(5)

* Draw 3 Constitutional isomers of

C_4H_8



(1)

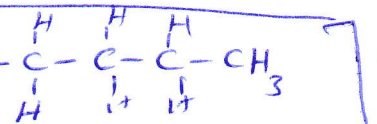


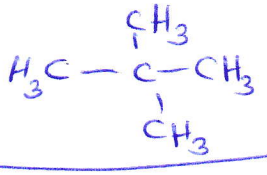
(2)

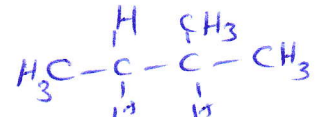
(3)

- Writing Structural formulas:-

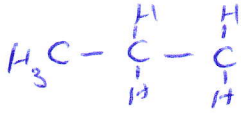
Ex1. C_5H_{12}

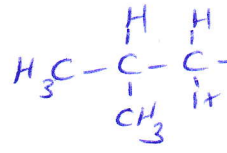
a) 

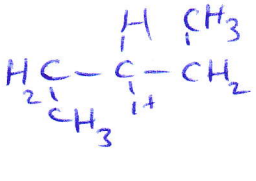
b) 

c) 

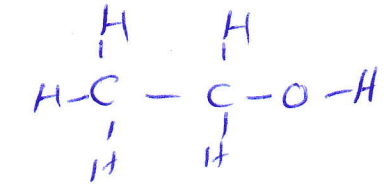
3 Constitutional isomers.





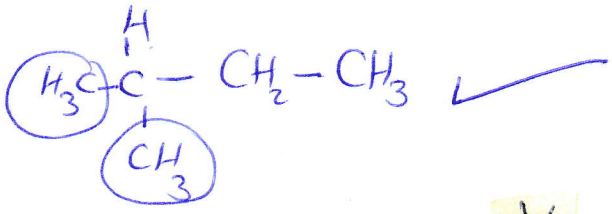


Abbreviated Structural formulas:

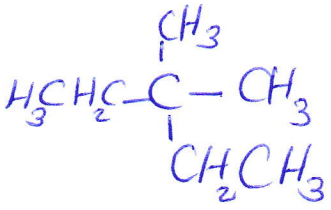
①  ≡ CH_3-CH_2-OH (CH_3CH_2OH)

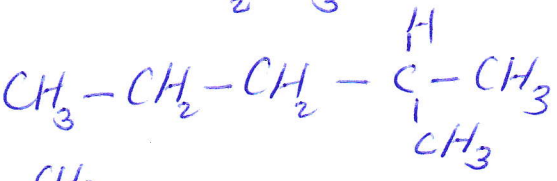
② $CH_3-CH_2-CH_2-CH_2-CH_3$ ≡ $CH_3-(CH_2)_3CH_3$

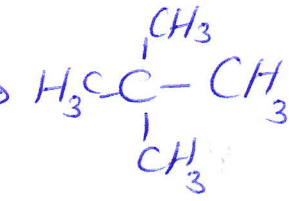
Expand the following formulai-

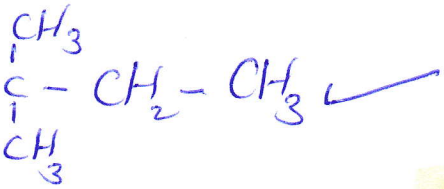
① $(CH_3)_2CH\ CH_2CH_3$ →  ✓

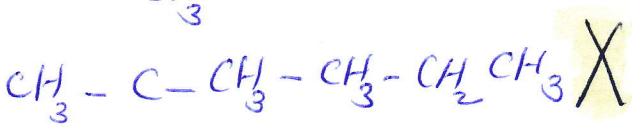
$CH_3-CH_3-CH-CH_2-CH_3$ ✗

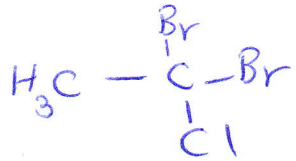
② $(CH_3CH_2)_2C(CH_3)_2$ → 

③ $CH_3(CH_2)_2CH(CH_3)_2$ → 

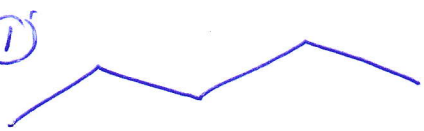
④ $(CH_3)_4C$ → 

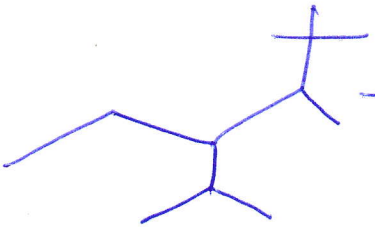
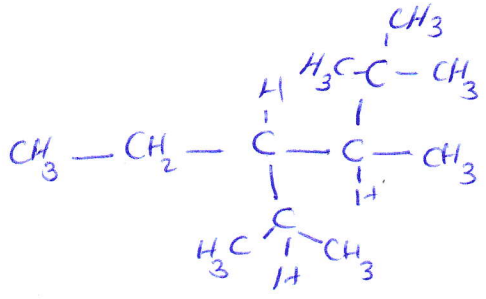
⑤ $CH_3\ C(CH_3)_2\ CH_2\ CH_3$ →  ✓

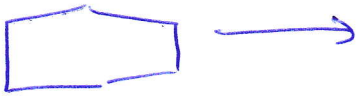
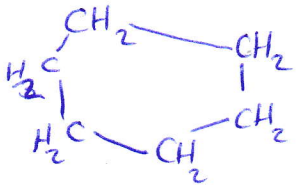
 ✗

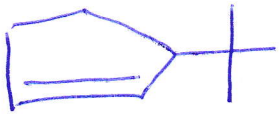
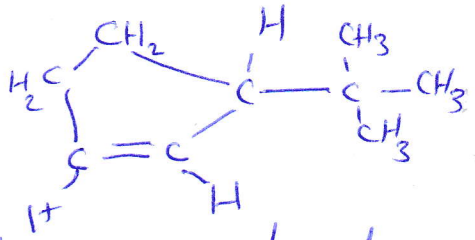
⑥ $CH_3\ CBr_2Cl$ → 

line bond formula

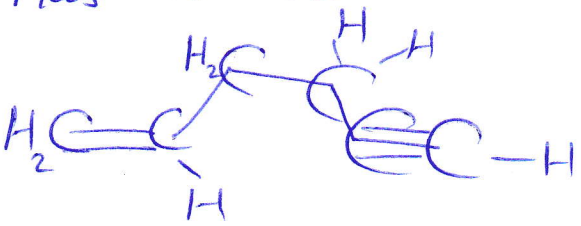
①  → $CH_3-CH_2-CH_2-CH_2-CH_3$

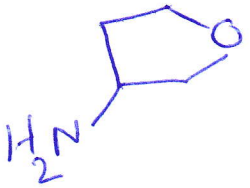
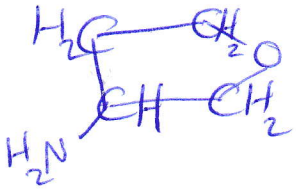
②  → 

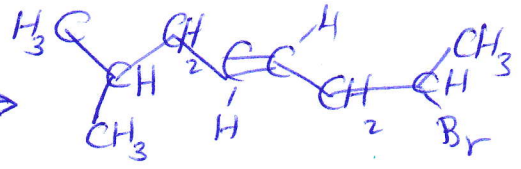
③  → 

④  → 

remember: each carbon has 4 bonds.

⑤  → 

⑥  → 

⑦  → 

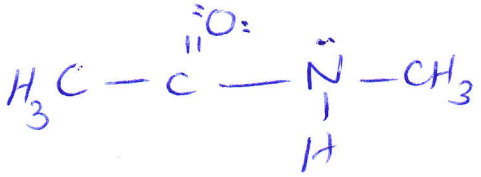
Find the molecular formula in each above example.

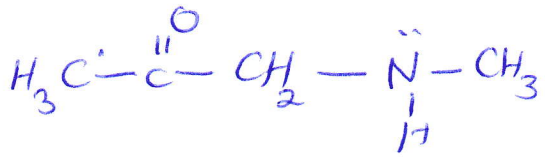
Functional group: certain arrangment of atoms.

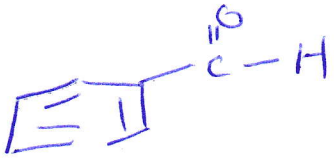
1. Only C–C and C–H ⟶ alkane
2. C=C ⟶ alkene
3. C≡C ⟶ alkyne
4.  ⟶ Arene "Aromatic"
5. C–X (X: halogen) ⟶ alkyl halide
6. C–OH ⟶ Alcohol
7. C–O–C ⟶ ether
8.  ⟶ Aldehyde
9.  ⟶ ketone
10.  ⟶ ester
11.  ⟶ Carboxylic acid
12.  ⟶ Amide
13.  ⟶ Amine
14. C–S–C ⟶ sulfide

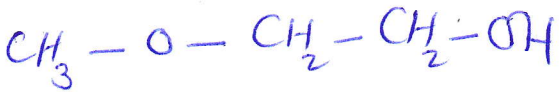
Now, go to specific examples.

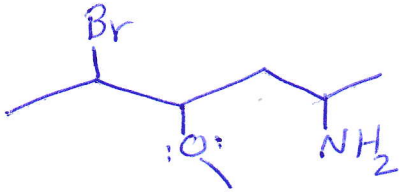
Find functional groups in each of the following structures?

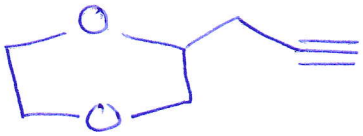


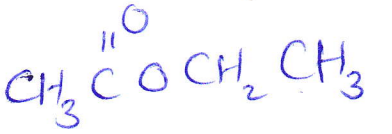


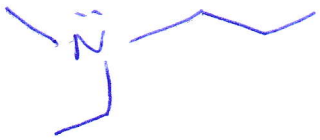












Also, in each molecule, write:

a) molecular formula
b) hybridization at each carbon
c) Bond angle at each carbon
d) Geometry for each carbon
e) Number of carbon-carbon double bond?

End of chapter 1.