Date:
19/10/2023

لجان الدُفعات

تفريغ عضويه 1

موضوع المحاضرة: Chpter (1+2)

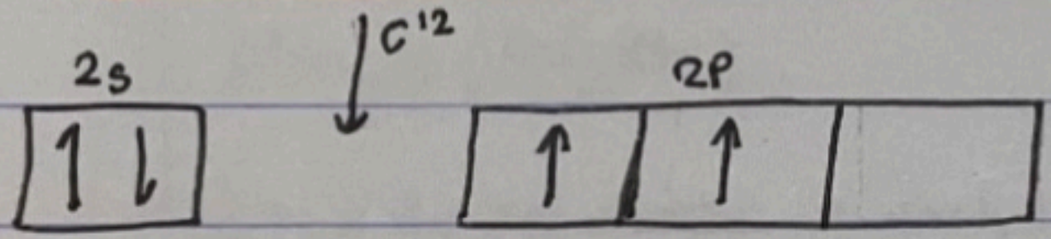
رقم المحاضرة : (2)

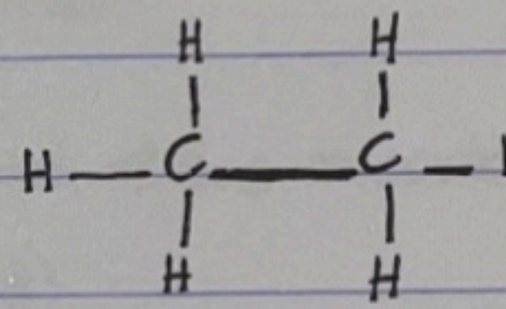
إعداد الصيدلانيه : Gufran Khaseed

Hyberidization : (the typs between S, P sharing ē) (new shape for orbital) (S energy < P energy)

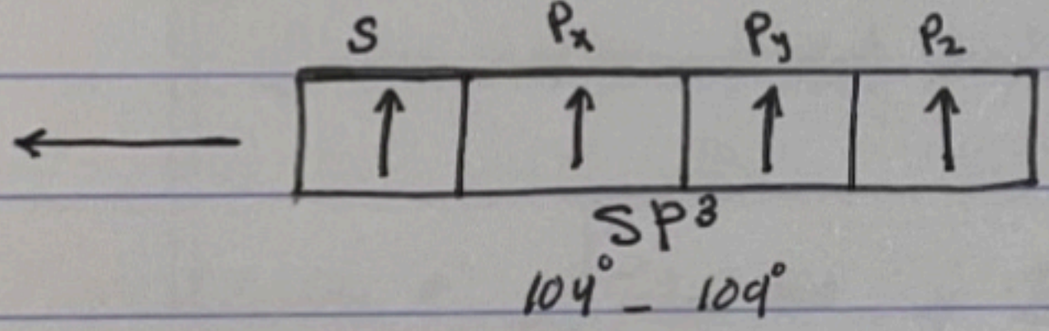
1) alkanes : (single bond) (sigma bond)

- sp3 (in level 2) → three 2p orbitals
  → 2 S orbitals
  → combined to form four new orbitals (hybrid orbitals) → required since there are four atoms attached to the central atom
- these new orbitals will have an energy slightly above the 2s orbitals and below the 2p orbitals (that no change occurred with the 1s orbital)
- Regular tetrahedron (shape) with all H_C_H bond angles of 109.5°
  ↑ the result of bonding 1S, P2

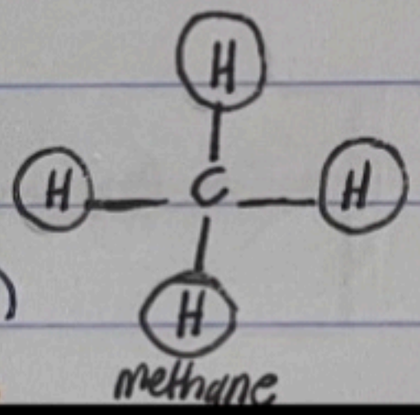




(have their specific shape)



104° _ 109°



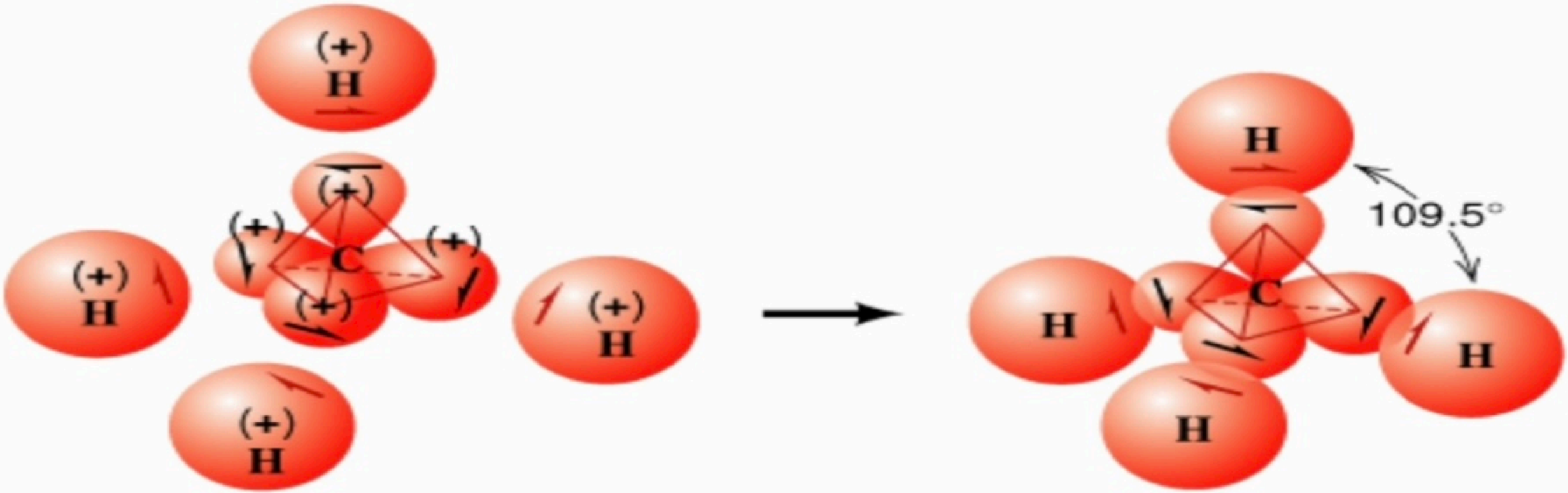
methane

(the angles and distance are necessary for energy stability)

+ slide 28.

note : H_C (يتكون) (تداخل الفلك S مع SP3.

Hybridization (Alkanes *sp3*)



Methane, CH_4

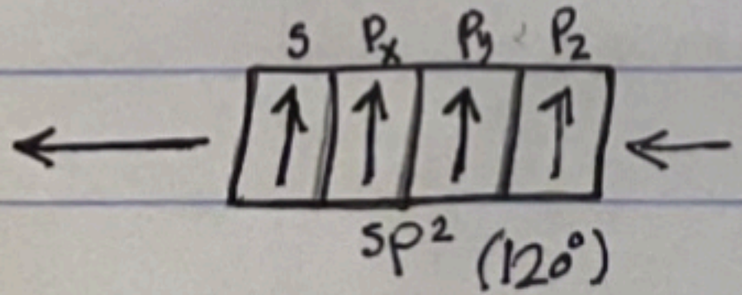
(في الصيدلية في التركيب)

② Alkenes : (double bond) (one sigma bond and one pi bond)

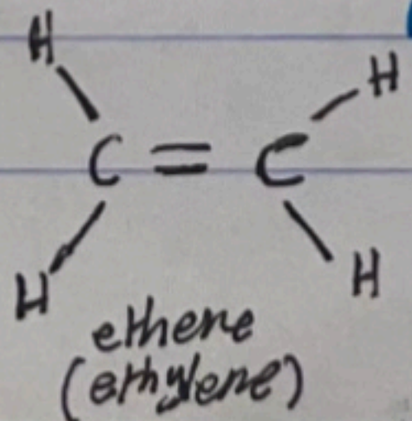
- sp2 → 2s orbitals (combined)
  - only two of 2p orbitals
  - Forming a three hybrid orbitals called sp_2 hybrid orbitals.

(since we only need 3 hybrid orbitals for the 3 groups, thinking of the groups as atoms and non-bonding pairs). Note:- the othe p-orbital (unhybridized)

- The trigonal planar arrangment has bond angles of 120° (at right angles)

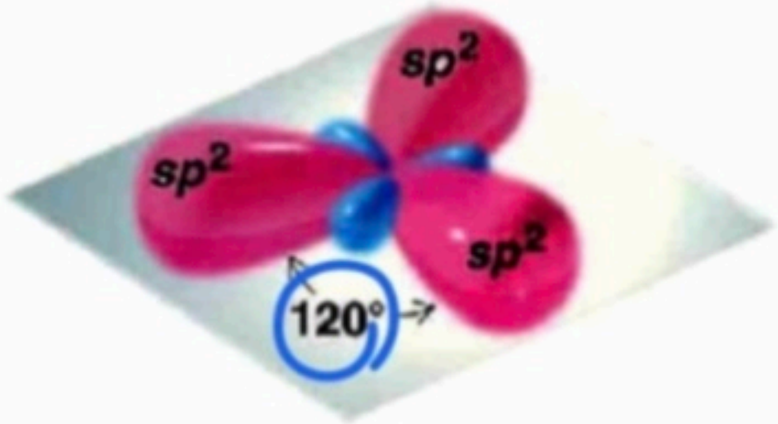


(in the trigonal planer arrangement of the hybrid orbitals)

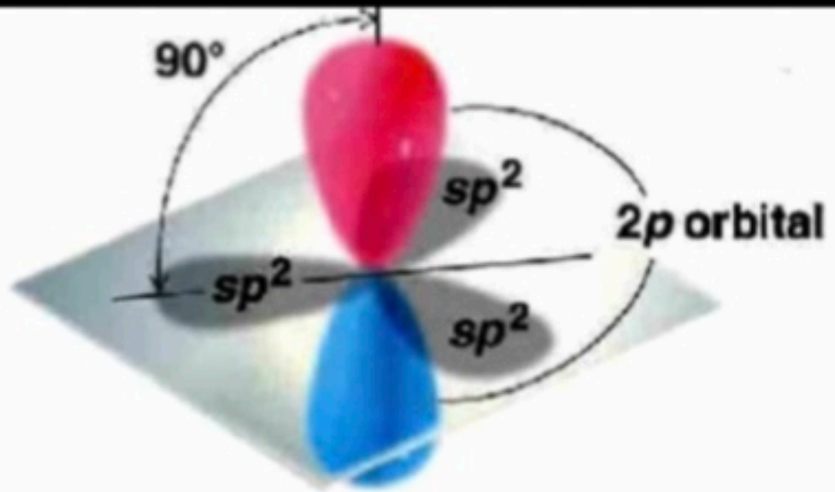


ethene
(ethylene)

(a) An sp^2 orbital



(b) Three sp^2 orbitals



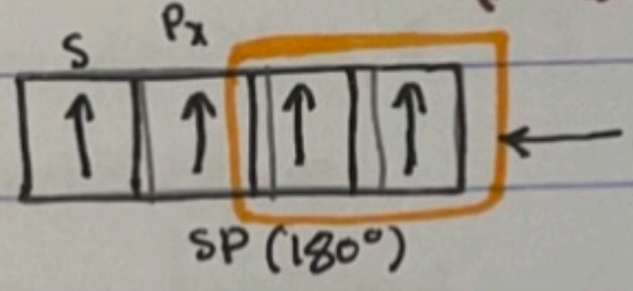
(c) Three sp^2 orbitals and an unhybridized 2*p* orbital

③ Alkynes: (3 bonds)

- case of → 2s orbitals
  sp → one of 2p orbitals.
  → it yield two sp (hybrid orbitals) → arranged as far apart as possible from each other → result → linear arrangement

- The Two unhybridized p- orbitals stay in they respective positions (at right angle of each other)

- linear molecule (180□) (liner because have a hard shap, harsh structure) (movment more difficult)



H — C ≡ C — H

Ethyne (Acetylene)

Formal charge: is the net charge on each atoms of the molecules or ions.

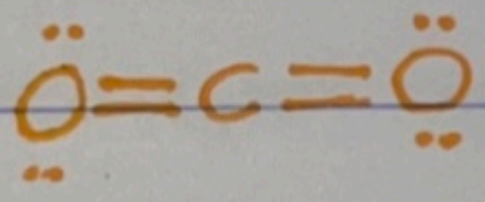
(which contain a covalent bond only)

$$\rightarrow FC = \text{Valence } e^- \text{ in free atom} - \left[\text{Total non bonding } e^- + \frac{\text{Total bonding } e^-}{2}\right]$$

ex: calculat the FC of CO_2:

FC for O = 6 - (4 + 4/2) = 0

FC for C = 4 - (0 + 8/2) = 0



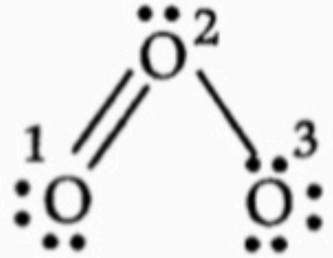
+slide 33, 34, 35

Formal Charge

Example :

The ozone

Lewis structure of O_3 is



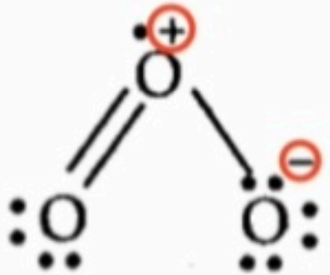
Formal charge on O(1) $= 6 - \left(4 + \frac{4}{2}\right) = 0$

Formal charge on O(2) $= 6 - \left(2 + \frac{6}{2}\right) = +1$

Formal charge on O(3) $= 6 - \left(6 + \frac{2}{2}\right) = -1$

+ net charge = zero

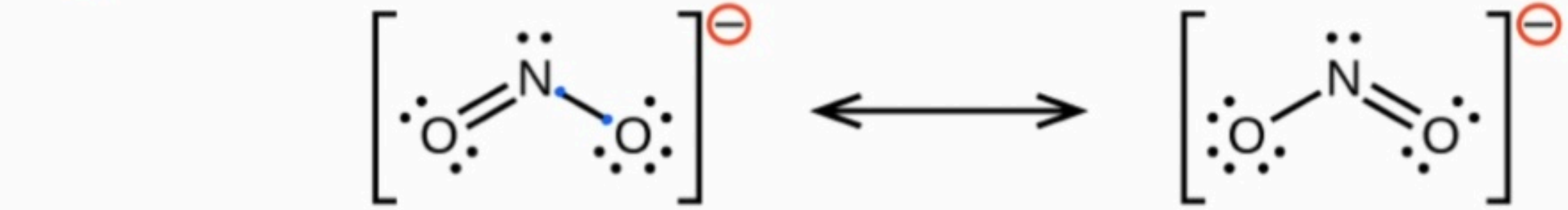
Hence we represent O_3 along with formal charges as follows.



slide 33

Formal Charge

Example :



Formal charge: 0 0 –1 –1 0 0

$O_1 \rightarrow 6-(4+\frac{4}{2})=0$

$O_2 \rightarrow 6-(6+\frac{2}{2})=-1$

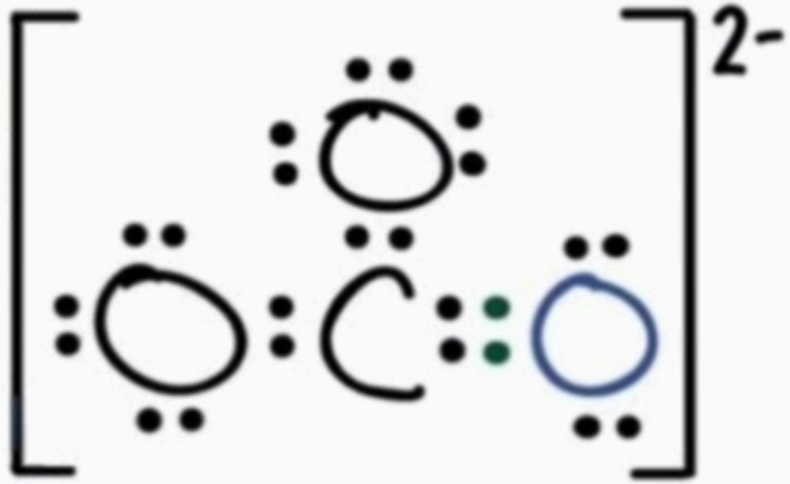
$N \rightarrow 5-(2+\frac{6}{2})=0$

slide 34

Formal Charge

Example :

CO_3^{2-}



Formal Charge	=	Valence Electrons	-	NonBonding Val Electrons	-	Bonding Electrons / 2		
C	=	4	-	0	-	8/2	=	0
O	=	6	-	6	-	2/2	=	-1
O	=	6	-	4	-	4/2	=	0

slide 35

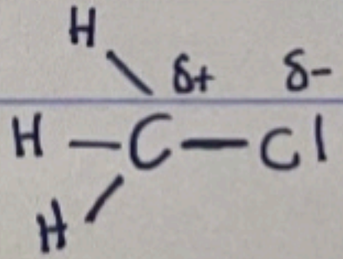
Inductive effect : the permenent displacment of electrons forming covalent bond (sigma σ bonds) towards the more electronegative element or group.

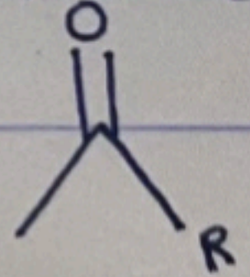
→ types : (symbols) ← represented by

1. electron - donating substituents **(+I)** : $-CH_3$, $-C_2H_5$

2. electron withdrawing substituents **(-I)** : $-NO_2$, $-CN$, $-SO_3H$, $-COOR$, $-NH_2$

$-OH$, $-OCH_3$ eg:- H_3C-Cl





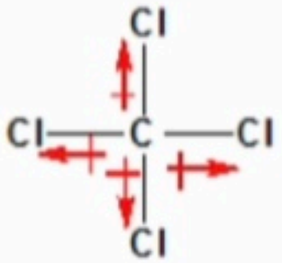
Bond Polarity and Dipole Moment

- **Dipole moment** (depends on the Inductiv effect).
- A bond with the electrons shared equally between two atoms is called a **nonpolar bond** like in Cl-Cl and C-C bond in ethane.
- A bond with the electrons shared unequally between two different elements is called a **polar bond**.
- The **bond polarity** is measured by its dipole moment (μ)
- **Dipole moment** (μ) defined to be the amount of charge separation (+δ and –δ) multiplied by the bond length.

Text

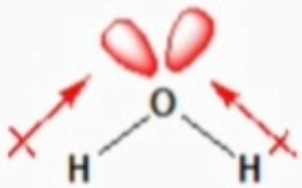
Partially

CCl_4



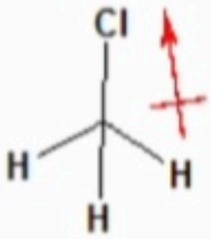
μ = zero

H_2O



μ ≠ zero

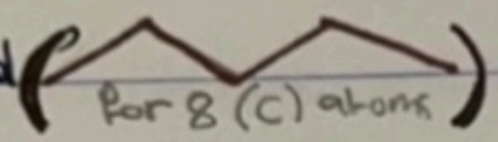
CH_3Cl

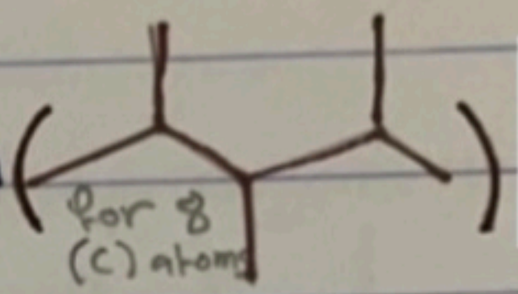


μ ≠ zero

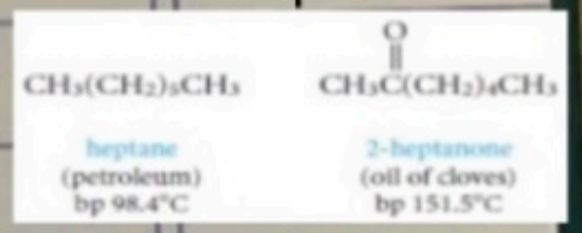
→ Classification according to molecular framework

1. acyclic compounds (not cyclic)

a. unbranched chains 

b. branched chains 

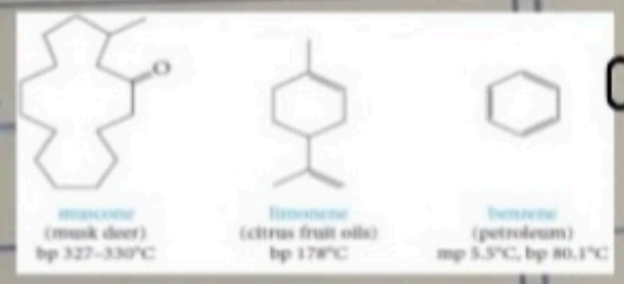
Cyclic examples



2. Carbocyclic compounds: Contain rings of Carbon atoms

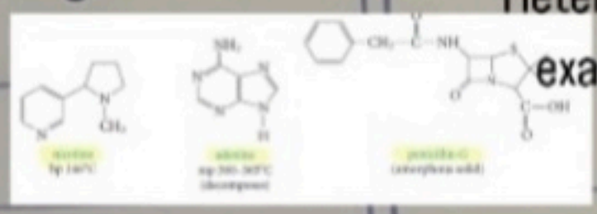
a. saturated b. unsaturated.

Carbocyclic examples



3. Heterocyclic compounds: it have at least one atom in the ring must be (heteroatom) → an atom that is not carbon eg: N.O.S ...)

Heterocyclic examples



→ Classification according to functional Group

is an arrangment of atoms with distinctive ← defined 1

physical and chemical properties.

is a reactive portion of an organic ← defined 2.

molecule, an atom, or a group of atoms that confers on the whole molecules it's characteristic properties.

slide 40, 41, 42, 43

Table 1.6 The Main Functional Groups

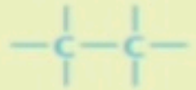
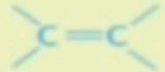
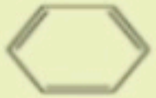
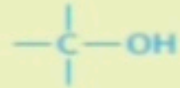
	Structure	Class of compound	Specific example	Common name of the specific example
A. Functional groups that are a part of the molecular framework				
acyclic		alkane	$CH_3—CH_3$	ethane, a component of natural gas
carbocyclic		alkene	$CH_2=CH_2$	ethylene, used to make polyethylene
heterocyclic		alkyne	$HC\equiv CH$	acetylene, used in welding
	(unbranched)			
		arene		benzene, raw material for polystyrene and phenol
B. Functional groups containing oxygen				
1. With carbon–oxygen single bonds		alcohol	CH_3CH_2OH	ethyl alcohol, found in beer, wines, and liquors
		ether	$CH_3CH_2OCH_2CH_3$	diethyl ether, once a common anesthetic

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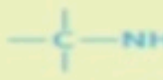
Table 1.6 — continued

	Structure	Class of compound	Specific example	Common name of the specific example
2 *With carbon–oxygen double bonds**		aldehyde	$CH_2{=}O$	formaldehyde, used to preserve biological specimens
		ketone	CH_3CCH_3 (O)	acetone, a solvent for varnish and rubber cement
3 *With single and double carbon–oxygen bonds*		carboxylic acid	$CH_3C{-}OH$ (O)	acetic acid, a component of vinegar
		ester	$CH_3C{-}OCH_2CH_3$ (O)	ethyl acetate, a solvent for nail polish and model airplane glue
*C. Functional groups containing nitrogen***		primary amine	$CH_3CH_2NH_2$	ethylamine, smells like ammonia
		nitrile	$CH_2{=}CH{-}C{\equiv}N$	acrylonitrile, raw material for making Orlon
D. Functional group with oxygen and nitrogen		primary amide	$H{-}C(=O){-}NH_2$	formamide, a softener for paper
E. Functional group with halogen group 7 with (c)	—X	alkyl or aryl halide	CH_3Cl	methyl chloride, refrigerant and local anesthetic
F. Functional groups containing sulfur†		thiol (also called mercaptan)	CH_3SH	methanethiol, has the odor of rotten cabbage
		thioether (also called sulfide)	$(CH_2{=}CHCH_2)_2S$	diallyl sulfide, has the odor of garlic

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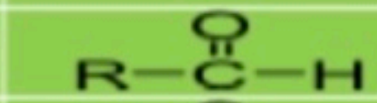
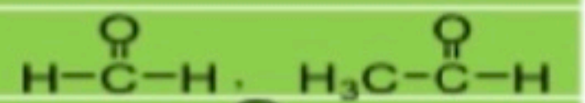
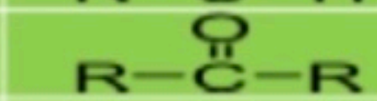
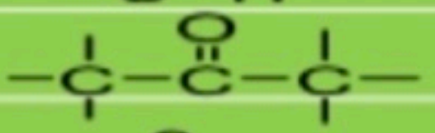
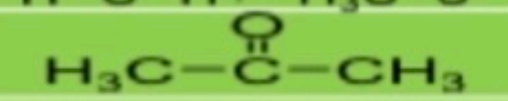
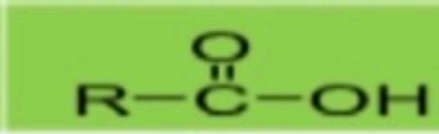
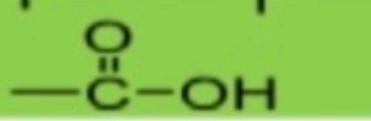
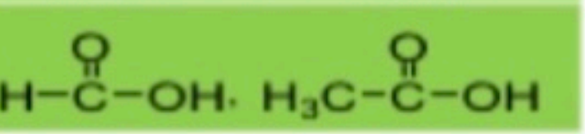
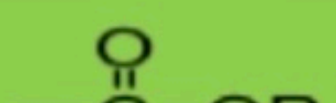
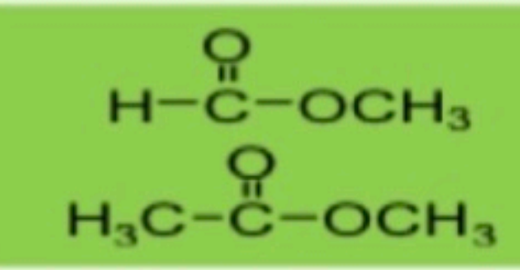
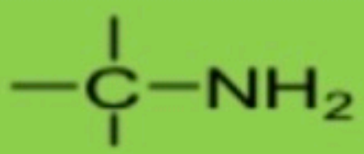
Functional Groups

Class	General formula	Functional group	Specific
Alkane	RH	C – C (single bond)	H3C – CH3
Alkene	R – CH = CH2	C = C (double bond)	H2C = CH2
Alkyne		 (triple bond)	
Alkyl halide	RX	-X (X = F, Cl, Br, I)	H3C - Cl
Alcohol	R – OH	-OH	H3C - OH
Ether	R – O –R’	- C- O – C -	H3C – O – CH3
Aldehyde			
Ketone			
Carboxylic acid			
Ester			
Amine	R – NH2		H3C – NH2

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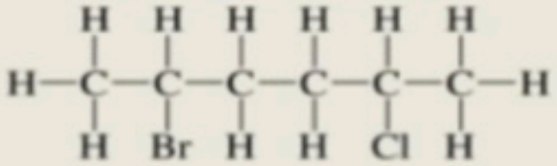
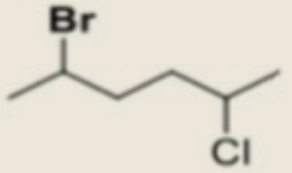
Dash formula

Kekul structur e | **Condensed structures** | **Bond line formula**

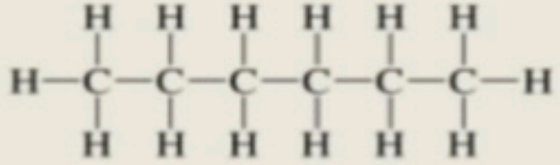
Atoms bonded to a carbon are shown to the right of the carbon. Atoms other than H can be shown hanging from the carbon.



$CH_3CHBrCH_2CH_2CHClCH_3$ or $CH_3CH(Br)CH_2CH_2CH(Cl)CH_3$

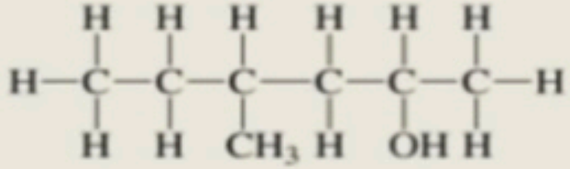


Repeating CH_2 groups can be shown in parentheses. بين قوسين

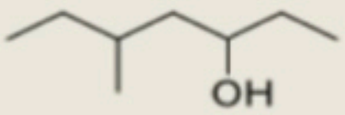


$CH_3CH_2CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_4CH_3$

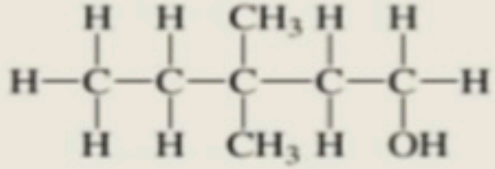
Groups bonded to a carbon can be shown (in parentheses) to the right of the carbon, or hanging from the carbon.



$CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$ or $CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$



Groups bonded to the far-right carbon are not put in parentheses



$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or $CH_3CH_2C(CH_3)_2CH_2CH_2OH$

slide 43

Chapter - 2 : Aliphatic Hydrocarbon

- Hydrocarbons / Aliphatic hydrocarbons :- organic compounds contain only the two elements Carbon and hydrogen.

1. Saturated hydrocarbons → Alkanes (C_nH_{2n+2}) (contain C - C single bond)
   → cycloAlkanes (C_nH_{2n}) (contain C - C sing bond in a single ring)

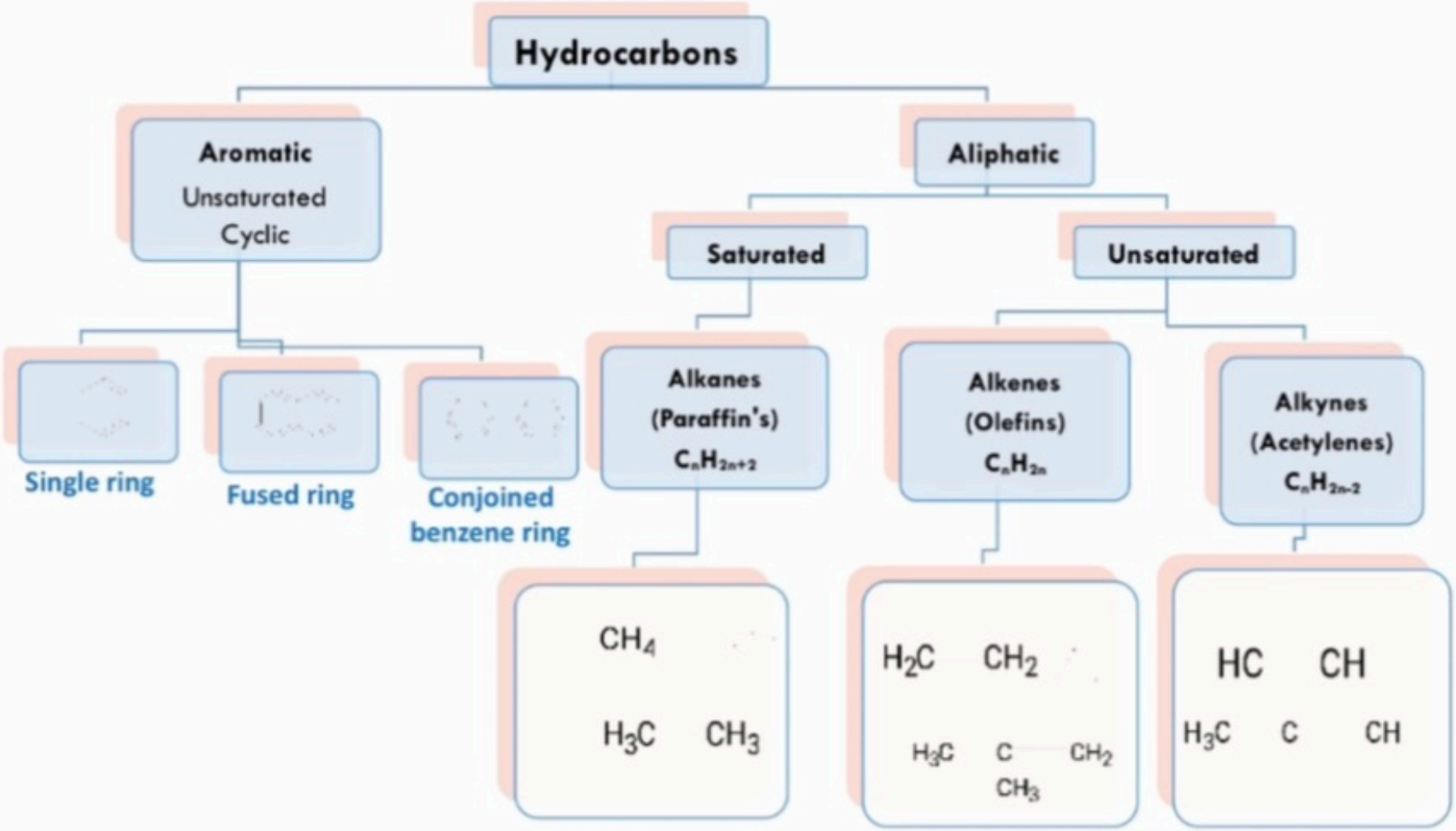
   are so similar that many of their properties can be considered side by side.

2. unsaturated hydrocarbons
   - AlKenes (C_nH_{2n}) (C=C)
   - AlKynes (C_nH_{2n-n}) (C≡C)

   ↳ it cyclic but the bonds unsaturated (the bond double, single, double, single ---) → orbitic discrimination تمييز

+ slide 3

Hydrocarbons



slide 3

saturated hydrocarbons:-

① Alkanes:-

- General formula (C_nH_{2n+2}) (one covalent bond)
- the four sp^3 orbitals of carbon ⟶ Tetrahedral arrangement
  bond angles of 109.5° like in CH_4 (methane) ↵
- C—H bond + slide 5

C (sp^3) — overlaps — H (1s)

حفظ

Saturated Hydrocarbons
1. Alkanes

Names, Molecular formulas and Number of Isomers of the first ten Alkanes

Name	Molecular Formula	Number of isomers
Methane alkane	CH_4	1
Ethane	C_2H_6	1
Propane	C_3H_8	1
Butane	C_4H_{10}	2
Pentane	C_5H_{12}	3
Hexane	C_6H_{14}	5
Heptane	C_7H_{16}	9
Octane	C_8H_{18}	18
Nonane	C_9H_{20}	35
Decane	$C_{10}H_{22}$	75

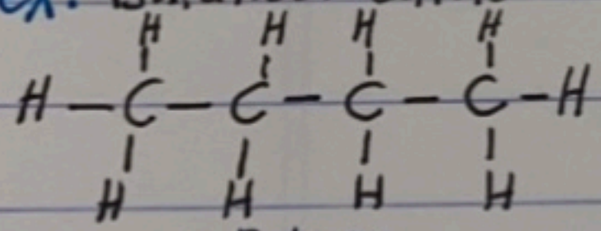
▲ structural isomerism.

→ Isomers : different compounds with identical molecular formulas

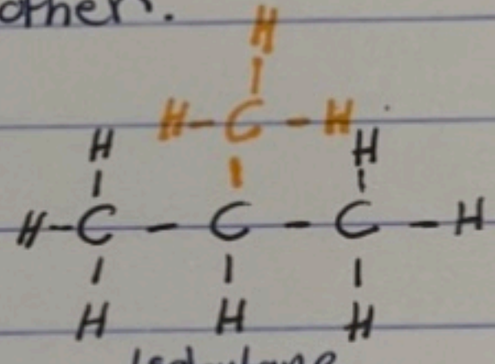
→ The phenomenon is called Isomerism

• The structural or constitional isomers which differ in the sequence (تسلسل) of atoms bonded to each other.

ex: Butanes. C_4H_{10}



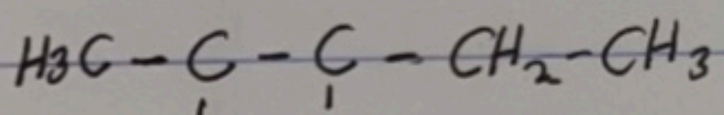
n-Butane



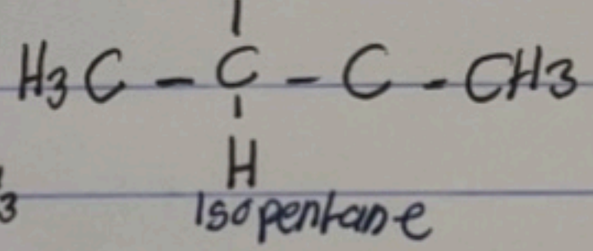
Isobutane

note: the one carbon compond havn't isomers.

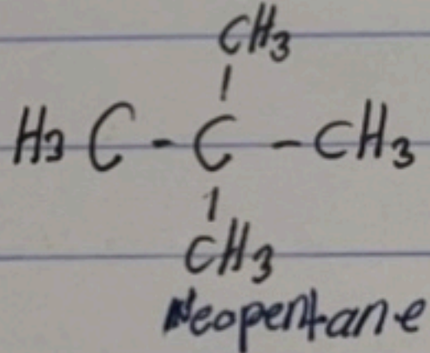
ex. pentanes, C_5H_{12}



n-pentane



Isopentane



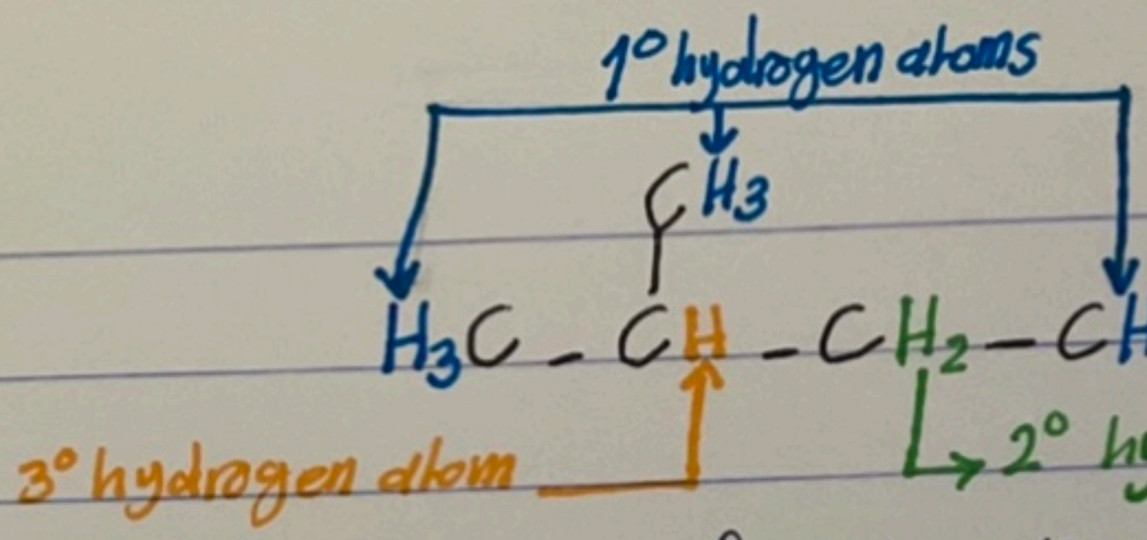
Neopentane

▲ classes of carbons and hydrogen:

→ primary carbon (1°): this one is bonded to only one othor carbon

→ secondry carbon (2°): this one is bonded to two other carbons

→ tertiary carbon (3°): this one is bonded to three other carbons



(Hydrogens are also referred as 1°, 2°, 3° according to the type of carbon they are bonded to)

→ Alkyl groups: an alkane from which a hydrogen has been removed

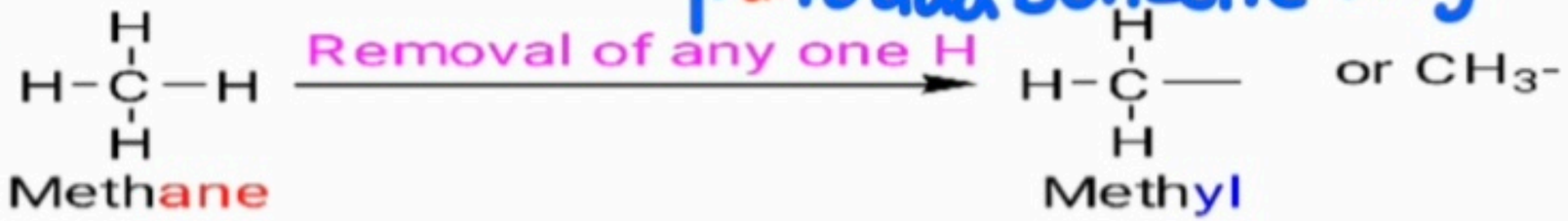
- General formula (C_nH_{2n+1}) represented by (R)
- nomenclature of alkyl groups:

replacing the suffix -ane of the parent alkane by -yl

i.e. Alkane - ane + yl = Alkyl

+ examples + slide 11

- Examples:
  - *Methane*



ex: to add benzene ring

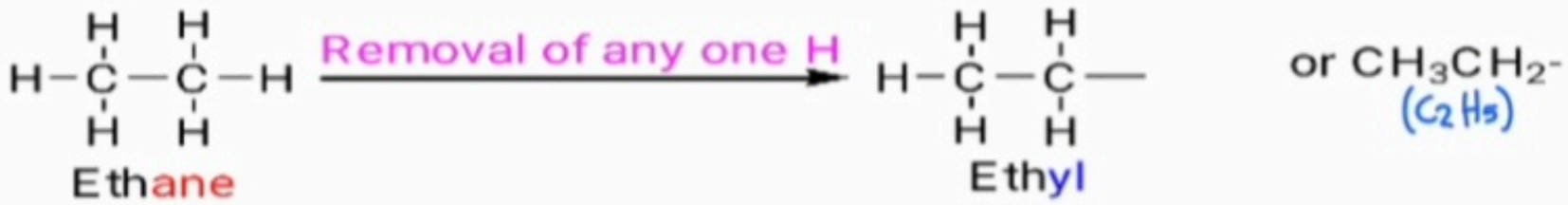
CH_3- (Methane – ane + yl) = methyl

Saturated Hydrocarbons

1. Alkanes

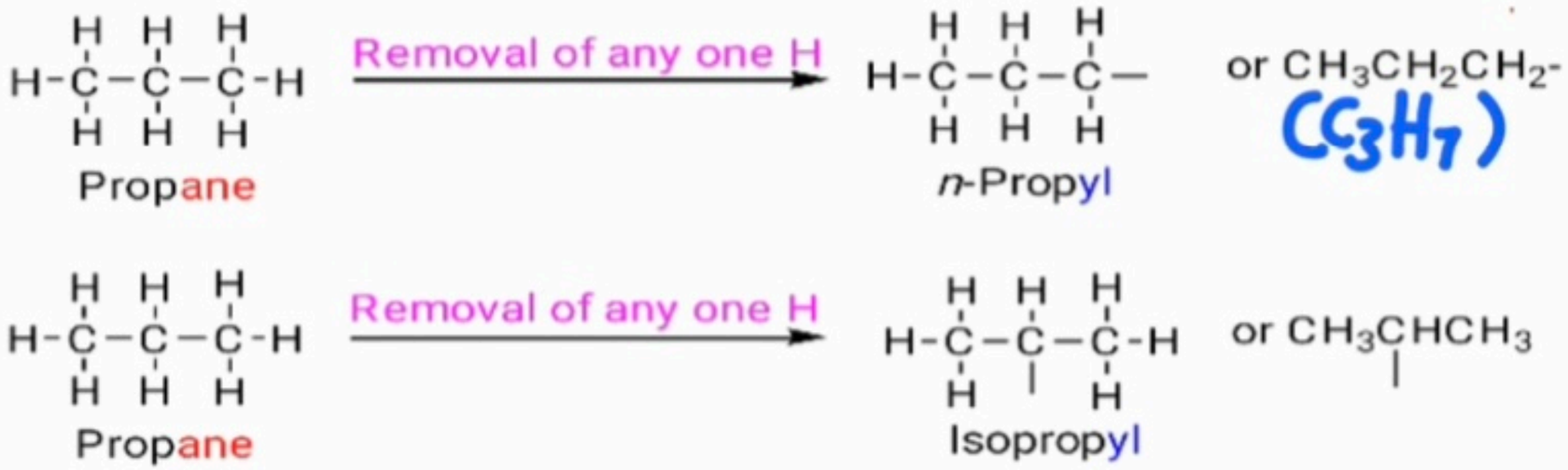
Alkyl Groups

- *Ethan*
  e (C_2H_6)



CH_3CH_2- (Ethane – ane + yl) = ethyl

- *Propane*
  (C_3H_8)



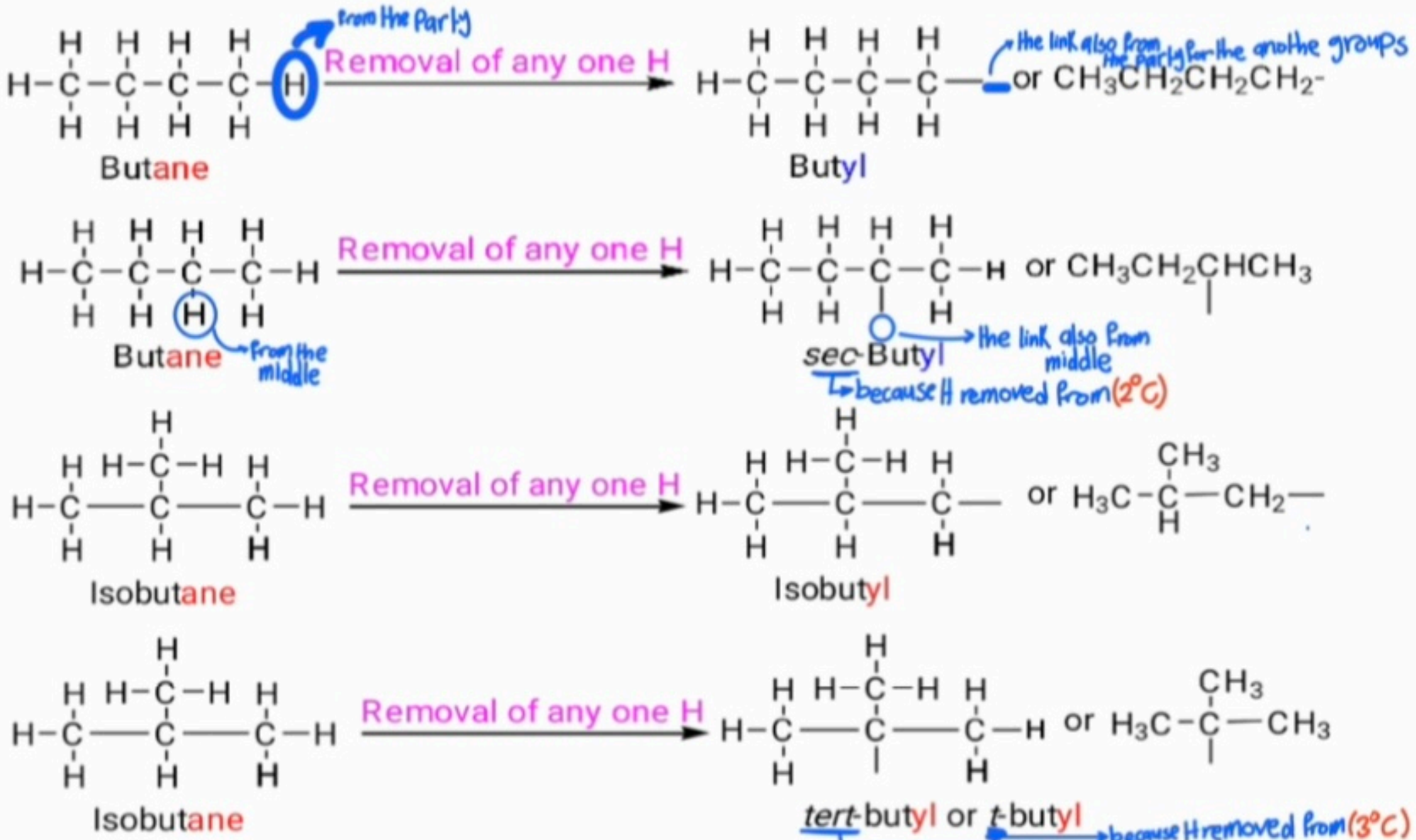
Propane – ane + yl = *n*-propyl or isopropyl

Saturated Hydrocarbons

1. Alkanes

Alkyl Groups

- *Butane*



Saturated Hydrocarbons

1. Alkanes

Alkyl Groups

Alkane		Alkyl Group	اختصار Abbreviation
$CH_3—H$ **Methane**	becomes	$CH_3—$ **Methyl**	Me–
$CH_3CH_2—H$ **Ethane**	becomes	$CH_3CH_2—$ **Ethyl**	Et–
$CH_3CH_2CH_2—H$ **Propane**	becomes	$CH_3CH_2CH_2—$ **Propyl**	Pr–
$CH_3CH_2CH_2CH_2—H$ **Butane**	becomes	$CH_3CH_2CH_2CH_2—$ **Butyl**	Bu–