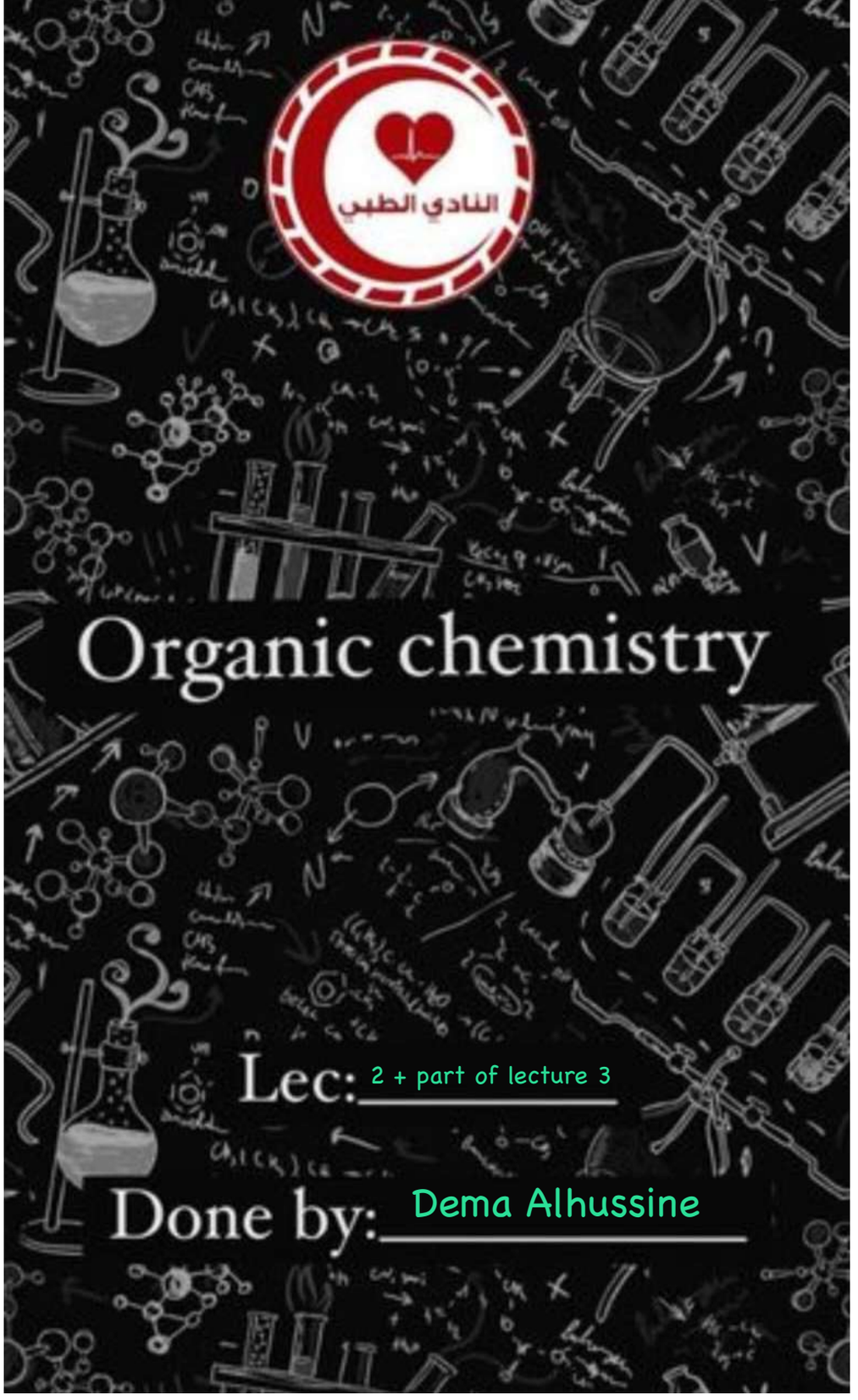


Organic chemistry

Lec: 2 + part of lecture 3

Done by: Dema Alhussine

Lewis Structures

It only deals with VE

Procedure for obtaining good Lewis structures: eg. CO_2

1) determine total number of valence shell e^- (including ionic charge if present).

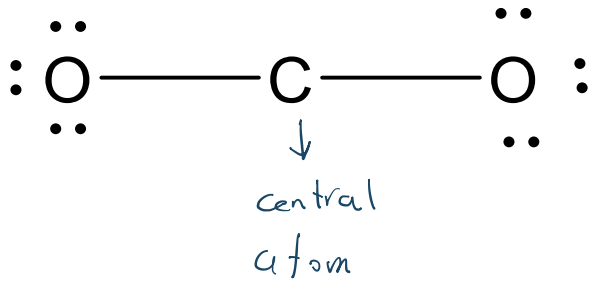
$$CO_2 = 4 + 2(6) = 16.$$

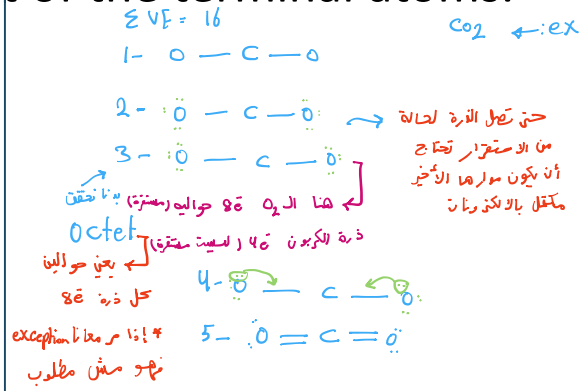
2) Chose a cental atom and draw a skeleton of the molecule connected with single bonds. (the central **atom** is usually the **least electronegative element** in the **molecule** or **ion**; hydrogen and the halogens are usually terminal.

O——C——O

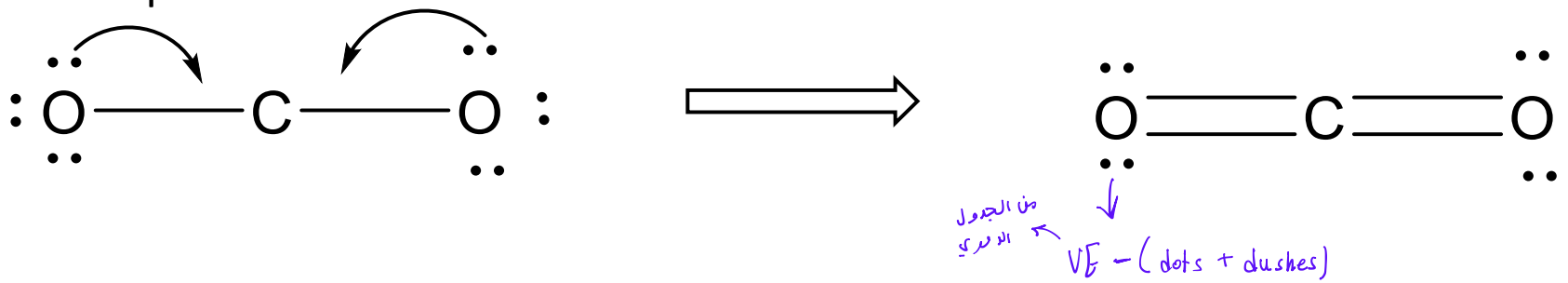
3) determine number of remaining e^-. complete the octet of the terminal atoms.

16 -4 = 12





4) Complete the octet Use lone pair e⁻ from terminal atoms to create multiple bonds.



5) determine the formal charges of all atoms.

Formal charge =
number of valence electrons – (number of lone pair electrons +1/2 number of bonding electrons)

For O 6-6 =0

For C 4-4 =0

معنى إشارة السالب أنه اكتسب الكترون

Ex: NO_3^- →

1. VE= 5+6*3+1 =24

VE(N) ← VE(O) عدد جزيئات الأوكسجين

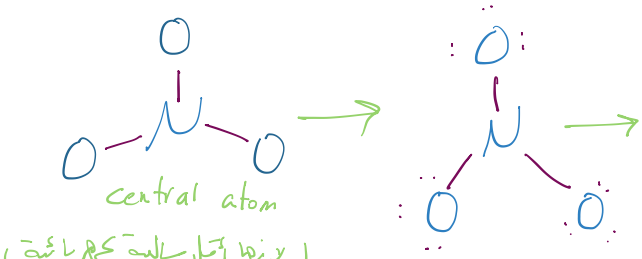
$5 + (6 * 3) + 1 = 24$

بنضيف بقدر مقدار الرقم بجانب الإشارة السالبة

---

* بنقص بقدر مقدار الرقم بجانب الإشارة الموجبة *

$24 - 6 = 18\ e^-$

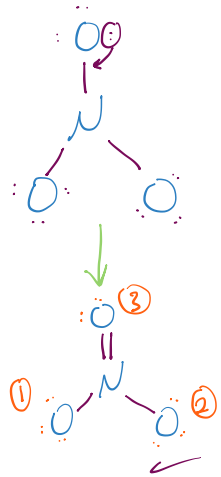


(لإنها أقل سالبية كهربائية)

الأوكسجين وصل مرحلة الاستقرار

النيتروجين بحاجة 2e ليصل لحالة الاستقرار

(incomplete octed)



* لازم لها أقل formal Charges

يطلع المجموع -1

① للأوكسجين ← $6-(6+1) = -1$

② للأوكسجين ← $6-(6+1) = -1$

③ للأوكسجين ← $6-(4+2) = 0$

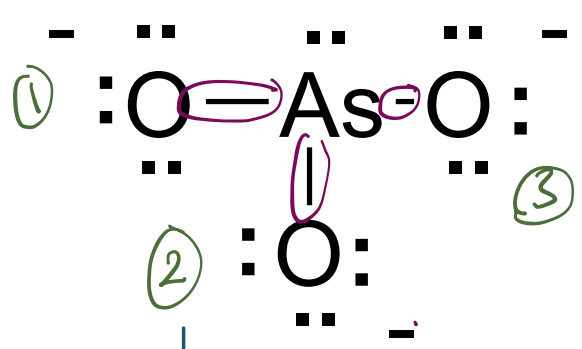
للنيتروجين ← $5-(0+4) = 1$

المجموع = -1 ✓

Lewis Structures (other examples)

Example 2: AsO_3^{3-}

1) # e^-: 5 + 3(6) + 3 = 26
2) form 3 single bonds
3) 20 e^- remain
4) O needs 6, As needs 2
5) All octets
6) Formal charges



As
5 − (2+3) = 0

1 أوكسجين
6 − (6+1) = −1

2 أوكسجين
6 − (6+1) = −1

3 أوكسجين
6 − (6+1) = −1

المجموع = −3

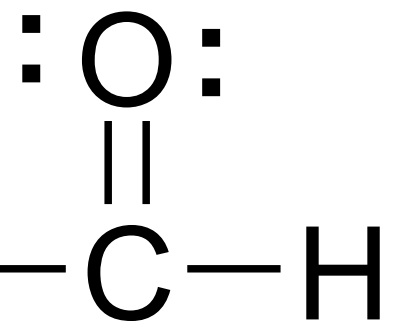
Lewis Structures (cont'd)

Example 3: CH_2O

4 1 6

C H O

1) # e^-: 4 + 2(1) + 6 = 12
2) try 3 single bonds
3) 6 e^- remain
4) O 6 but C?
5) Form a double bond
6) Both O & C octets
7) Formal charges



H → 1 − (0 + 1) = 0

C → 4 − (0 + 4) = 0

O → 6 − (4 + 2) = 0

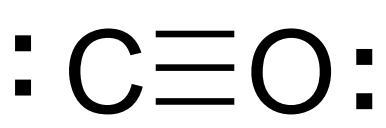
Σ formal charge = zero ✓

Lewis Structures (cont'd)

Example 4: CO

1) # e^-: 4 + 6 = 10
2) try 1 single bond
3) 8 e^- remain
4) C needs 6 as does O short 4 e^-
5) Share 4 more e^- - triple bond
6) Octets
7) Formal charges

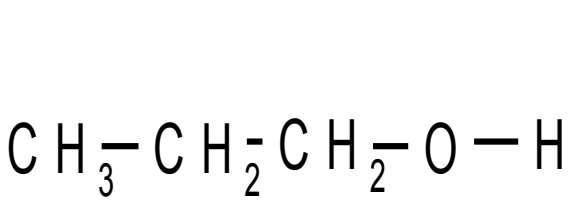
-1 +1



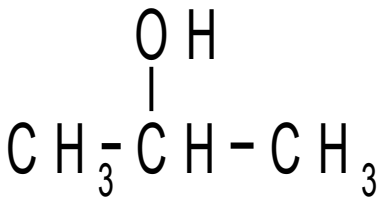
1.8 Isomers

Structural or **constitutional** isomers have same molecular formula but different structural formula.

They have different physical and chemical properties:



1-propanol
(bp 97.4 C)



2-propanol
(bp 82.4 C)

1.9 Writing Structural Formulas

write out all possible structural formulas that correspond to the molecular formula C_5H_{12}.

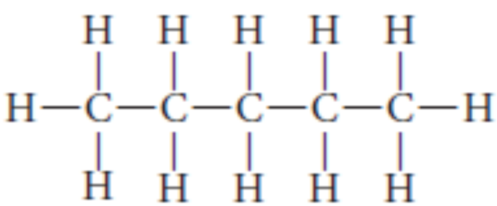
Structural Isomers لما بدي أرسم

C - C - C -C - C

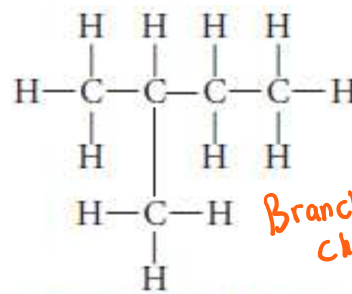
Continuous chain

C - C -C – C
      |
      C

Branched chain



pentane, bp 36°C



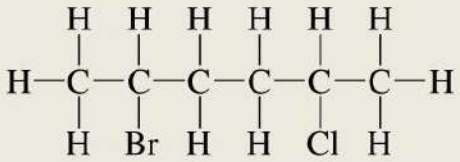
2-methylbutane, bp 28°C
(isopentane)

C forms 4 covalent bonds

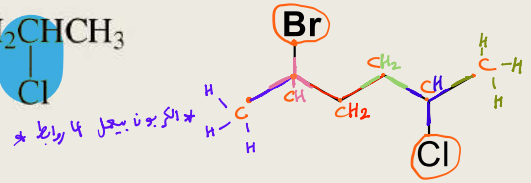
How to write the structural formula

Dash formula

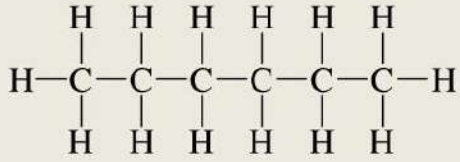
Kekul structure — Atoms bonded to a carbon are shown to the right of the carbon. Atoms other than H can be shown hanging from the carbon.



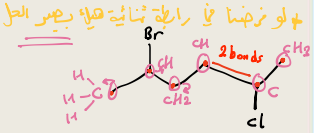
$CH_3CHBrCH_2CH_2CHClCH_3$ or $CH_3CH(Br)CH_2CH_2CH(Cl)CH_3$



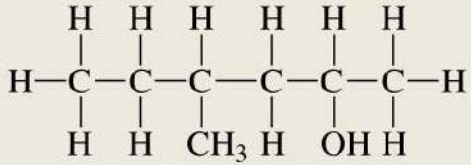
Repeating CH_2 groups can be shown in parentheses.



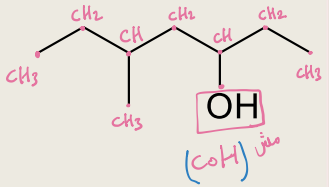
$CH_3CH_2CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_4CH_3$



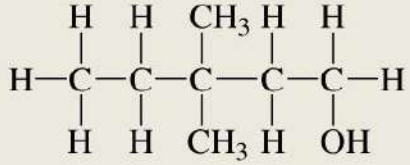
Groups bonded to a carbon can be shown (in parentheses) to the right of the carbon, or hanging from the carbon.



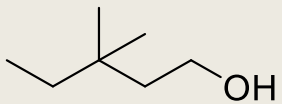
$CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$ or $CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$



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



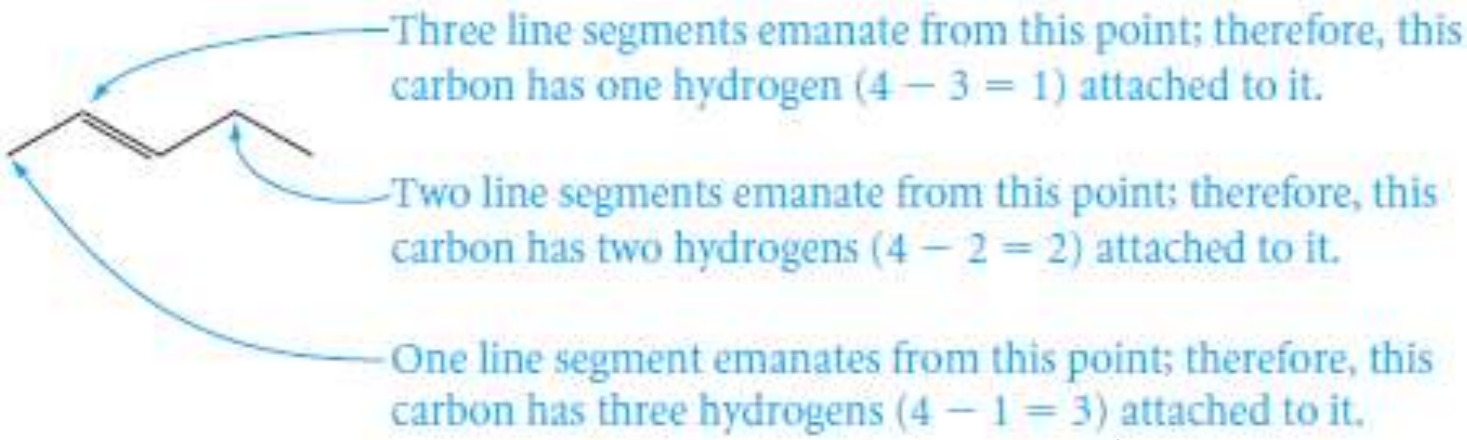
$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or $CH_3CH_2C(CH_3)_2CH_2CH_2OH$



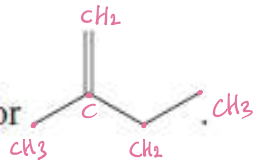
Condensed structures

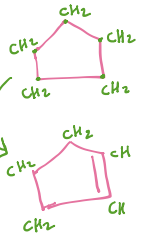
Bond line formula

$CH_3CH{=}CHCH_2CH_3$

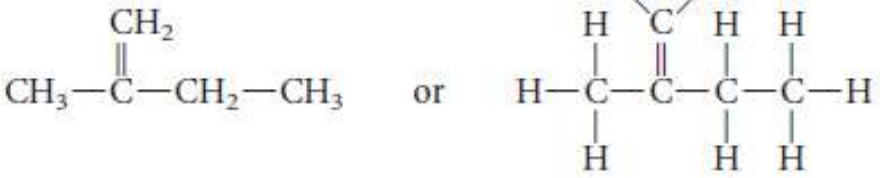


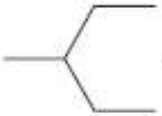
EXAMPLE 1.12

Write a more detailed structural formula for 



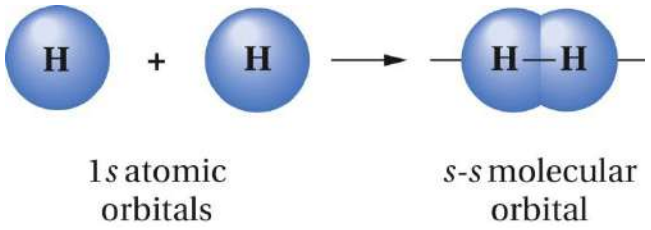
Solution

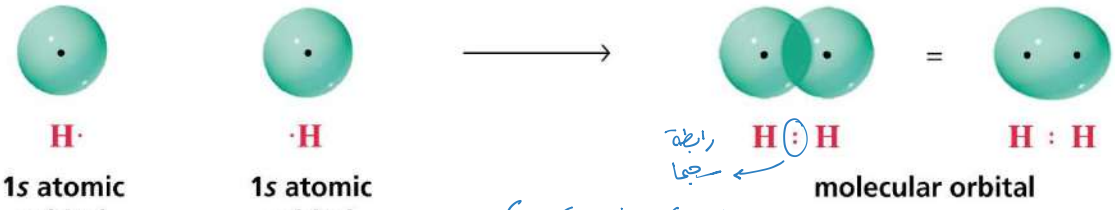


PROBLEM 1.23 Write a more detailed structural formula for  .

1.14 The Orbital View of Bonding; the Sigma Bond

Sigma (σ) bonds: are characterized by a region of high e⁻ density along the internuclear axis.





بدي أعمل تداخل بين ال orbital

Head to head / تداخل صبا ش

ممكن تكون بينا

أهم يكون في منطقة تداخل حقيقية

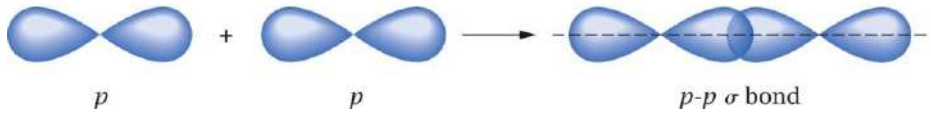
s – s

p – p

p – s

أو hybridized orbitals

حتى أكون ال Covalent bond



Orbitals approach each other in a **head to head** fashion

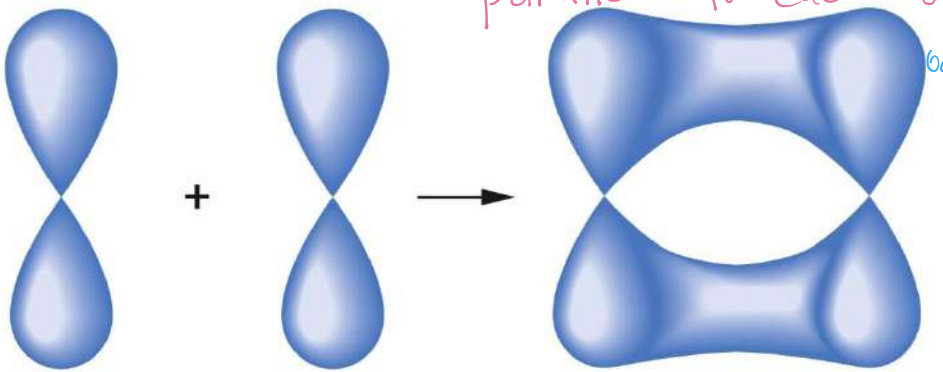
1.14 The Orbital View of Bonding; the pi (π) bond

There is one other type of bond, a pi (π) bond. In contrast to a sigma bond the e^- density in a pi bond is not located on the internuclear axis, but rather on either "side" of it.

Head to head وليس

π bonds are formed by the **side to side overlap** of 2 "p" orbitals

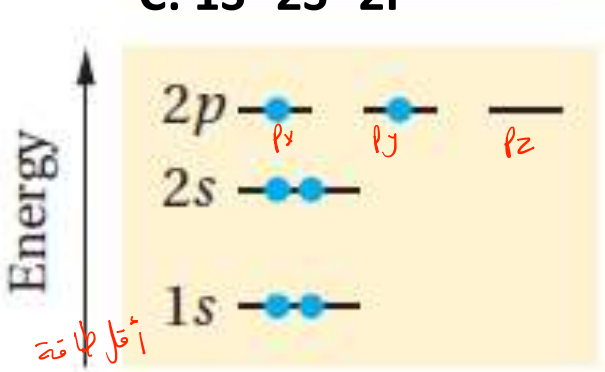
parallel to each other



p *p* π bond

Carbon sp^3 Hybrid Orbitals

^6C: $1S^2\ 2S^2\ 2P^2$

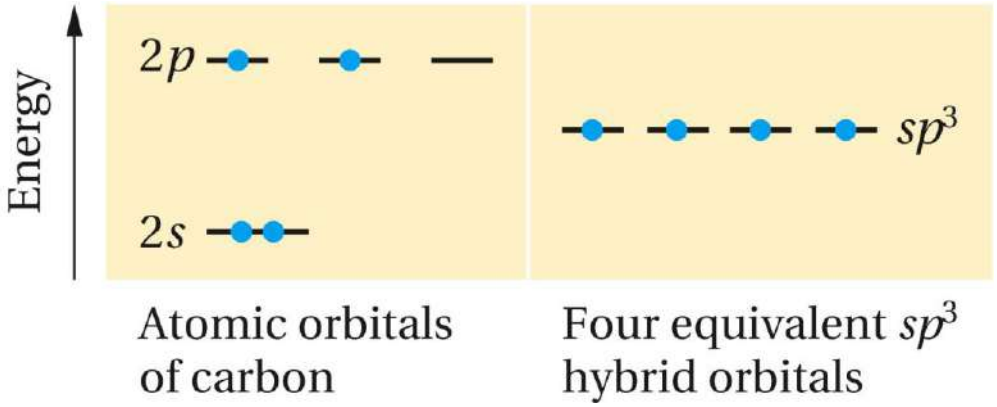


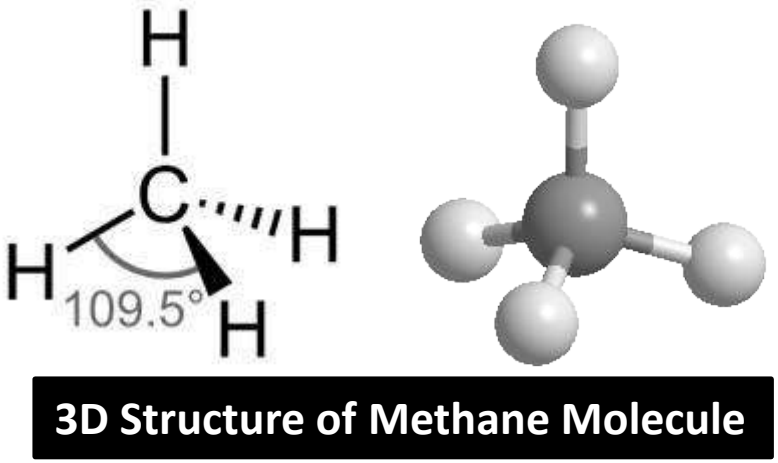
Distribution of the six electrons in a carbon atom. Each dot stands for an electron.

Q: Should the carbon form only two bonds !!!

A: We know from experience that carbon usually forms *four* single bonds, and often these bonds are all equivalent, as in CH_4

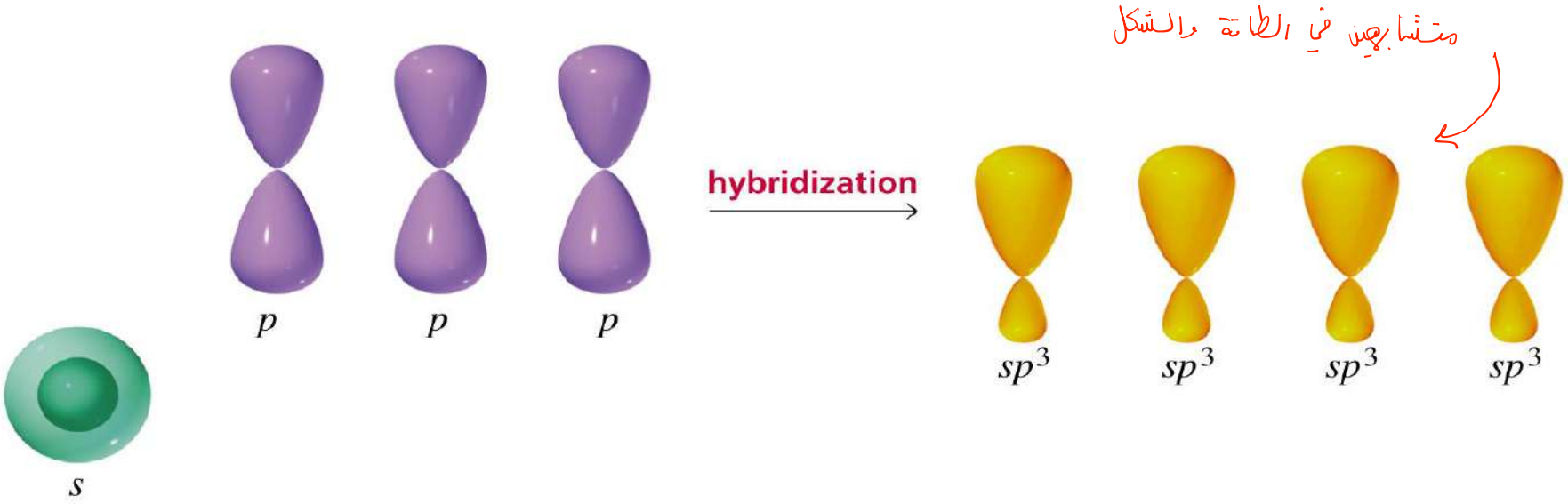
متساوية
قياس الزاوية + length
109.5°

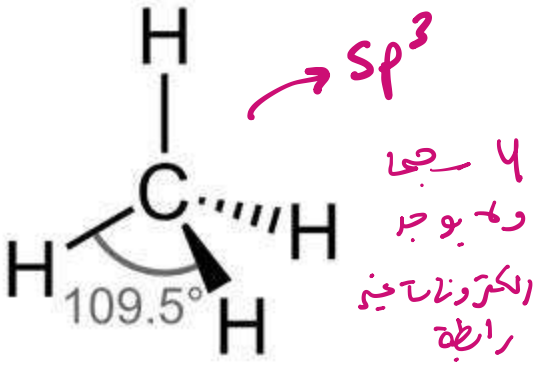


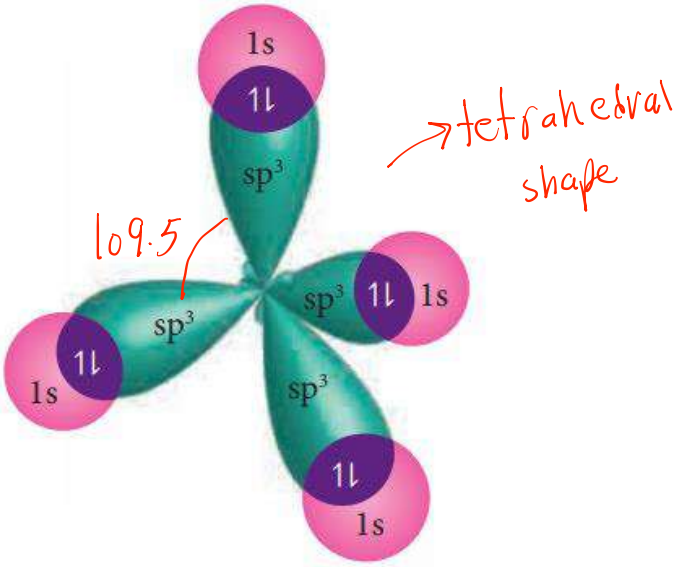


3D Structure of Methane Molecule

Mix or combine the four atomic orbitals of the valence shell to form four identical hybrid orbitals

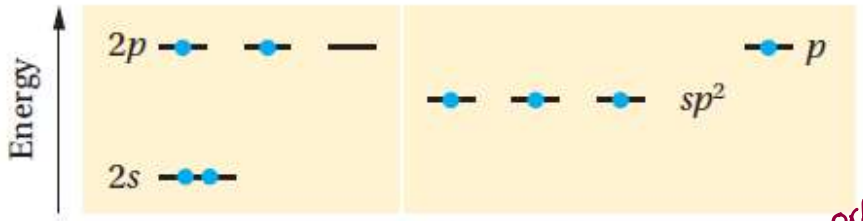






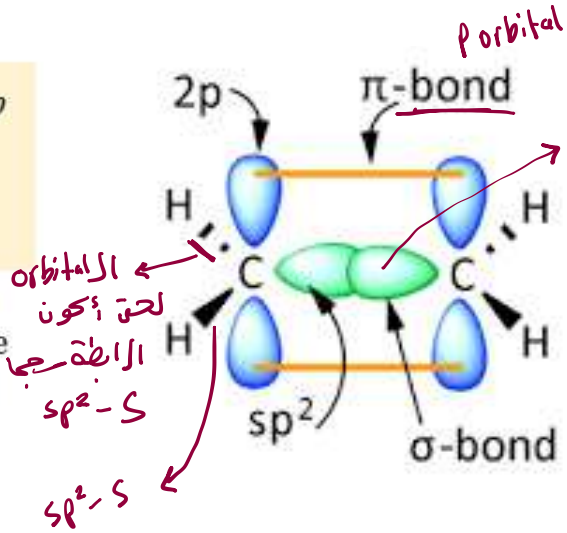
SP^2-Hybridized orbitals

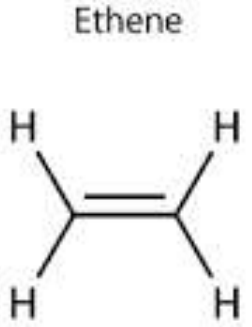
One part *s* and two parts *p* in character and are directed toward the three vertices of an equilateral triangle.

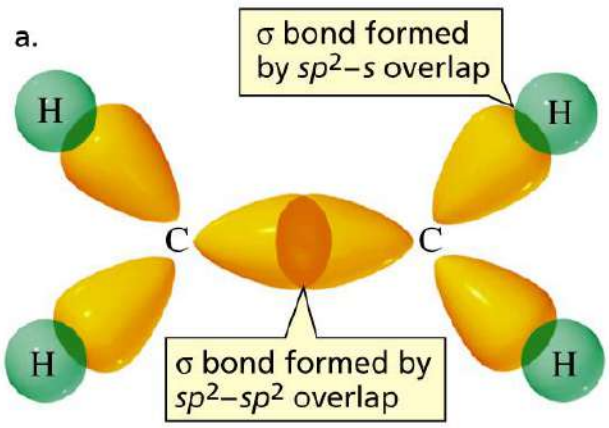


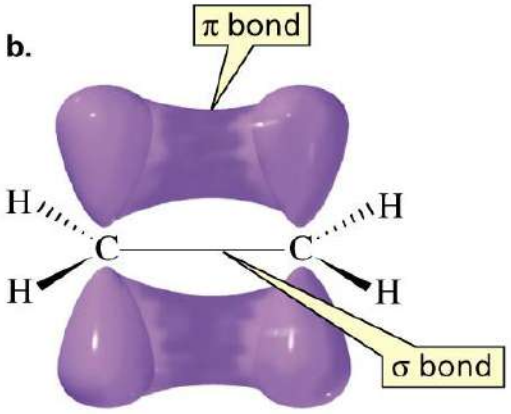
Atomic orbitals of carbon

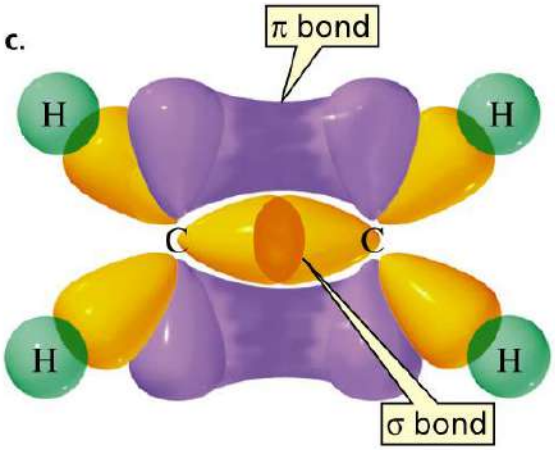
The 2*s* and two 2*p* orbitals are combined to form three hybrid sp^2 orbitals, leaving one electron still in a *p* orbital.







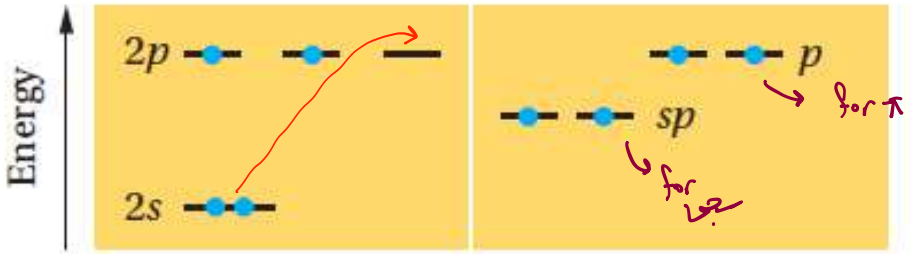




SP-Hybridized orbitals

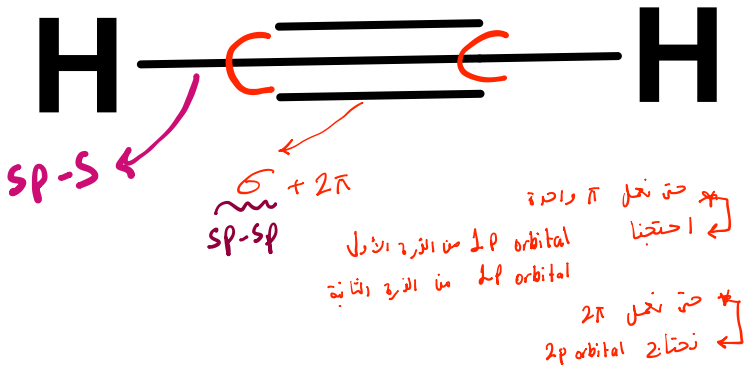
Bonding in Ethyne: **A Triple Bond**

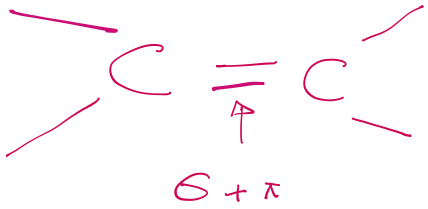
- A triple bond consists of one σ bond and two π bonds

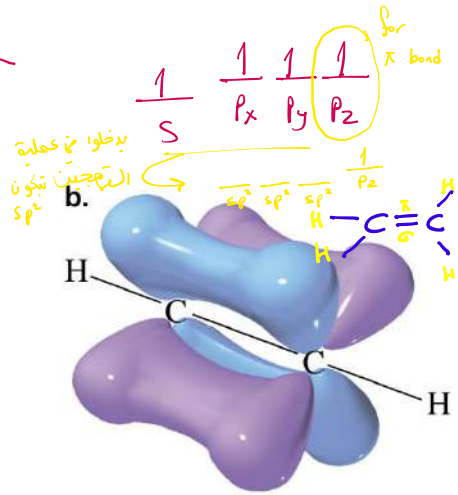


Atomic orbitals of carbon

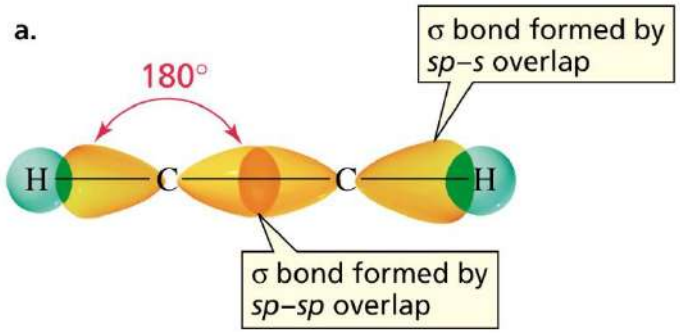
The 2*s* and one 2*p* orbital are combined to form two hybrid *sp* orbitals, leaving one electron in each of two *p* orbitals.







sp orbitals forms a sigma bond between the two carbons, and lateral overlap of the properly aligned *p* orbitals forms two pi bonds



Monday 4-3-2024

Valence Bond Theory (cont'd)

Orbitals are combined in various portions to make equivalent hybrid orbitals, *i.e.*

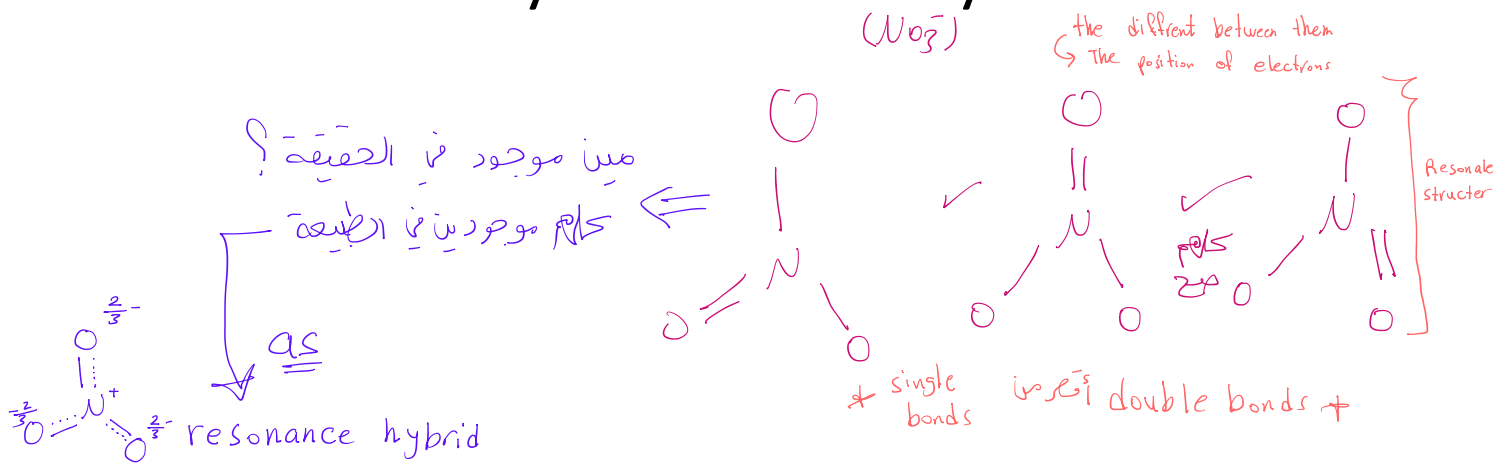
AOs(#(s, p))	hybrid	Angle	orientation
1, 1	2 sp	180^o	linear
1, 2	3 sp^2	120^o	trigonal planar
1, 3	4 sp^3	109^o	tetrahedral

1.12 Resonance

There are molecules (or ions) for which more than one correct Lewis structure can be drawn, these equivalent Lewis structures are resonance structures.

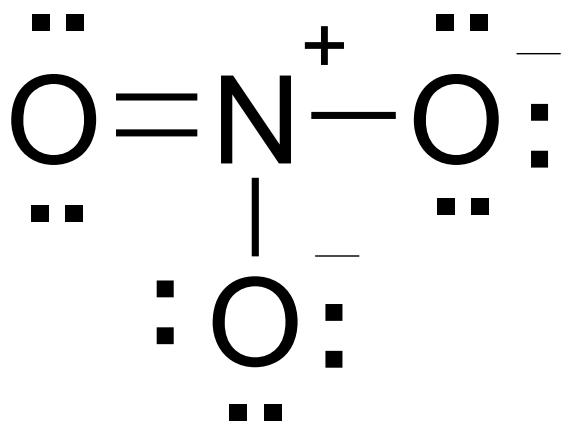
The assumption in these diagrams is that the atom positions do not change, we are only allowed to change the distribution of e^-, *i.e.* the bonds and lone pairs.

Lewis structures do not always explain properties of molecules. Resonance theory is a second layered approach.



Resonance (cont'd)

Example 1: NO_3^-

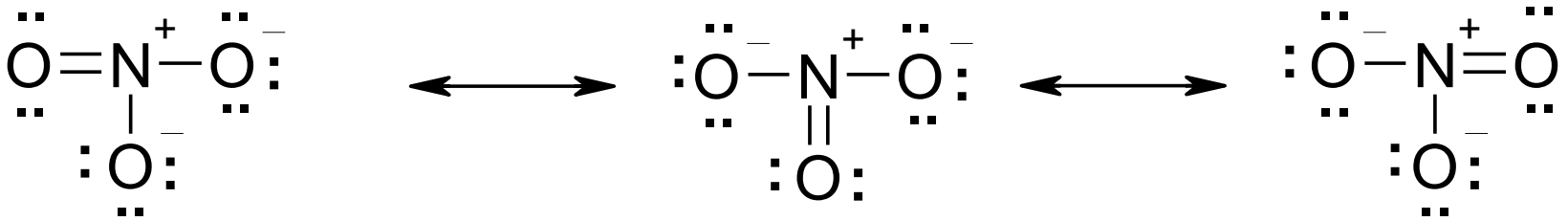


1) # e^-: 5 + 3(6) + 1 = 24
2) try 3 single bonds
3) 18 e^- remain
4) Each O needs 6, leave 2 short
5) Share 1 pair but which one?
6) Pick one O, octets
7) Formal chargall es

Resonance (cont'd)

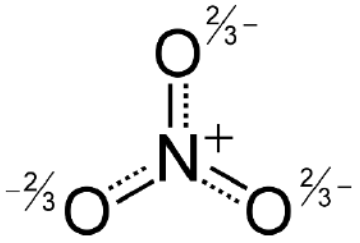
Example 1: NO_3^- (cont'd)

Depending on your choice of the double bond to oxygen, there are three possible structures differing in the location of the double bond and charges on the oxygen.



A B C

In real the structure is hybrid of all (A, B and C)



A **resonance hybrid**

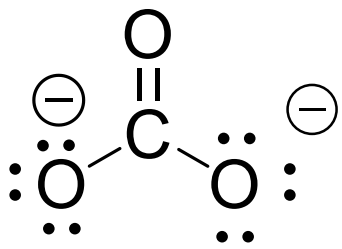
The Lewis structure can be converted to other by changing the position of electrons

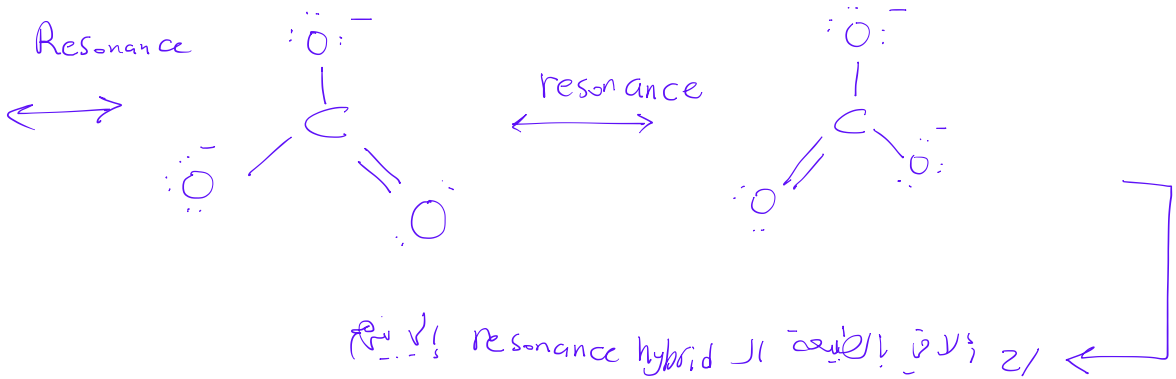
Rules for drawing resonance structures :

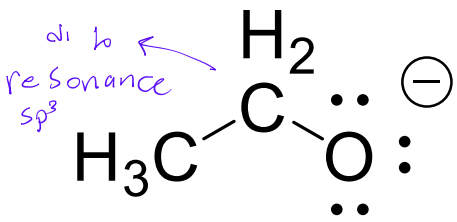
1) Electrons only can be oved (lone pair / π electrons)

2) Electrons move toward SP/ SP^2 hybridized atom only.

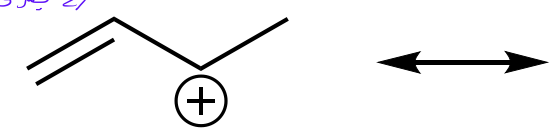
Examples: Write a second resonance structure for the following compounds?







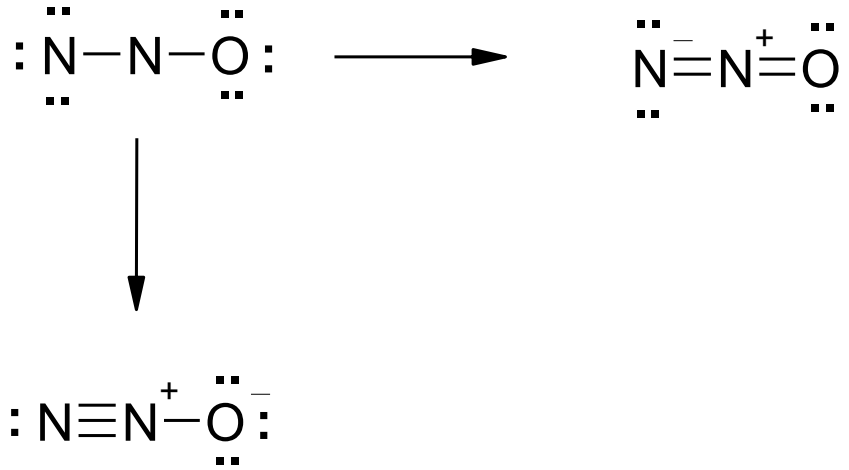
Exercise



Resonance (cont'd)

Example 2: N_2O

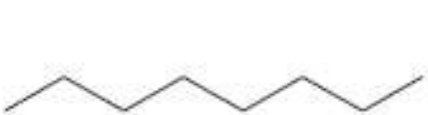
1) # e^-: 2(5) + 6 = 16
2) try 2 single bonds
3) 12 e^- remain
4) 16 e- for octets – 4 short
5) Options – 2 double bonds, 1 triple & 1 single
6) Octets
7) Formal charges
8) Which is better and why?



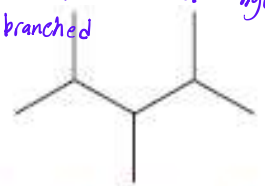
1.17: Classification According to Molecular Framework

- The three main classes of molecular frameworks for organic structures are **acyclic**, **carbocyclic**, and **heterocyclic** compounds.

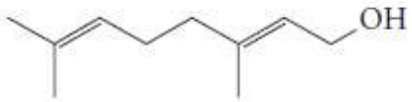
1.17.a Acyclic Compounds (*not cyclic*): contain chains that may be **unbranched** or **branched**.



unbranched chain of eight carbon atoms



branched chain of eight carbon atoms



geraniol
(oil of roses)
bp 229–230°C

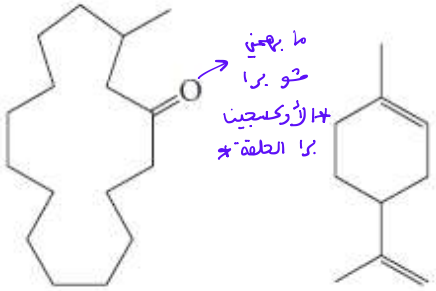
$CH_3(CH_2)_5CH_3$

heptane
(petroleum)
bp 98.4°C

$CH_3C(=O)(CH_2)_4CH_3$

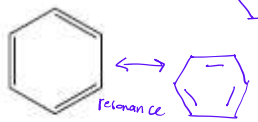
2-heptanone
(oil of cloves)
bp 151.5°C

1.17b: Carbocyclic Compounds: contain rings of carbon atoms



muscone
(musk deer)
bp 327–330°C

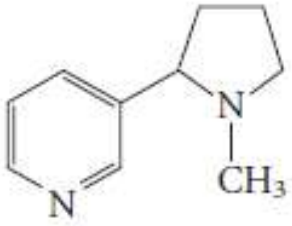
limonene
(citrus fruit oils)
bp 178°C



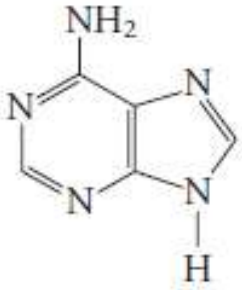
benzene
(petroleum)
mp 5.5°C, bp 80.1°C

1.17.c Heterocyclic Compounds (In heterocyclic compounds, at least one atom in the ring must be a heteroatom, an atom that is *not* carbon: *eg*. N, O,S...)

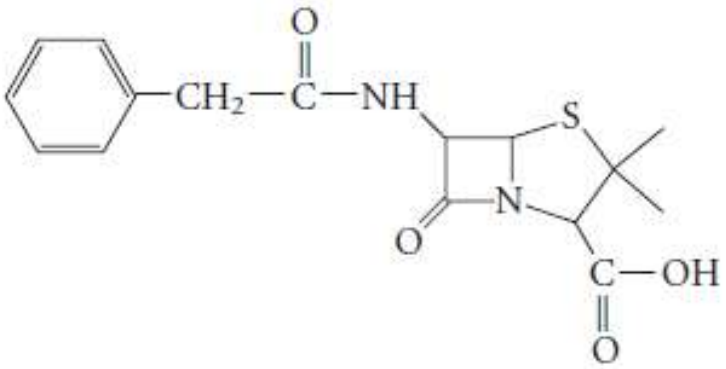
يتم استبدال واحدة من الكربون بذرة أخرى عادة لا S, O,
other atom



nicotine
bp 246°C



adenine
mp 360–365°C
(decomposes)



penicillin-G
(amorphous solid)

يعني مثلا البنزين لو شلت منه كربون وحطيت لا
Heterocyclic Compounds عائلة تحت المركب هاد

Classification According to Functional Group

A functional group is an arrangement of atoms with distinctive **physical** and **chemical** properties.

Table 1.6 The Main Functional Groups

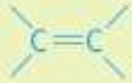
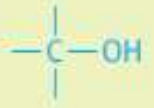
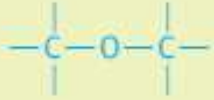
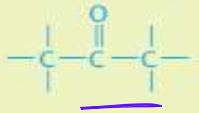
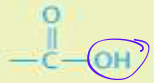
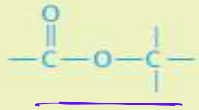
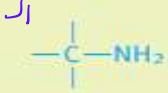
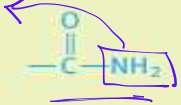
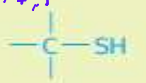
	Structure	Class of compound	Specific example	Common name of the specific example
A. Functional groups that are a part of the molecular framework		alkane	$CH_3—CH_3$	ethane, a component of natural gas
		alkene	$CH_2=CH_2$	ethylene, used to make polyethylene
		alkyne	$HC\equiv CH$	acetylene, used in welding
		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

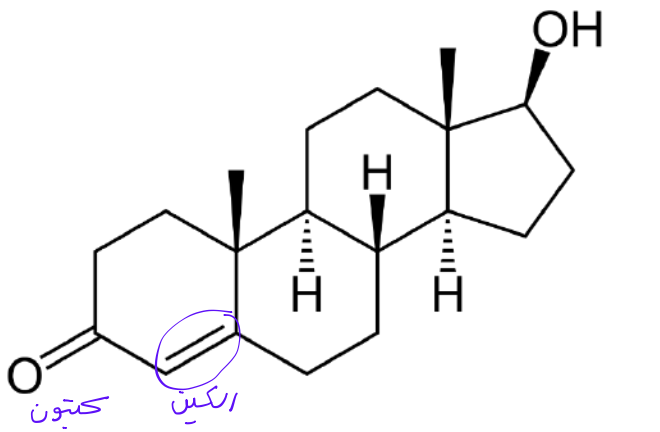
Table 1.6 continued

	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	$CH_3C(=O)OH$	acetic acid, a component of vinegar
		ester	$CH_3C(=O)OCH_2CH_3$	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		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

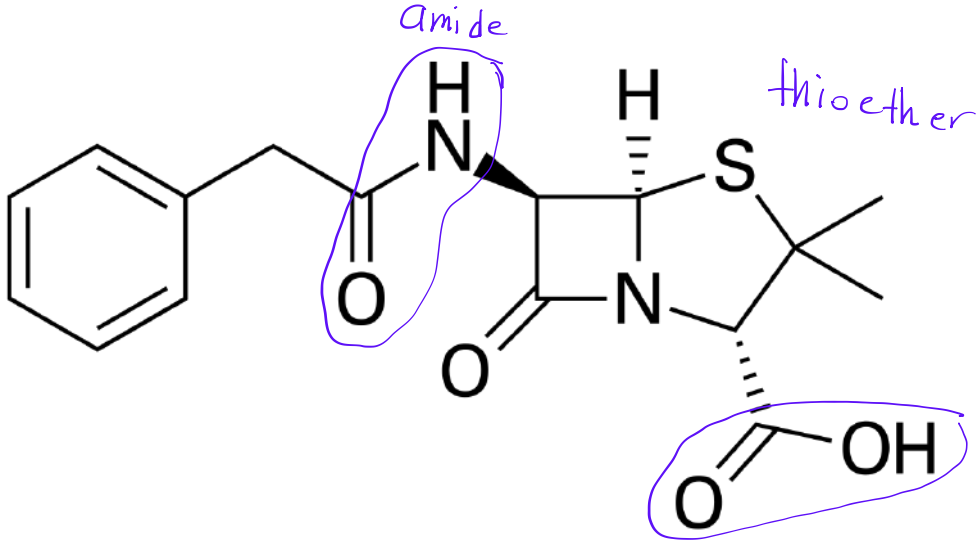
Ex. What functional groups can you find in the following natural products?

لـ ← اذكر اسم العائلة

عائلة الكحول



testosterone



penicillin-G

Karboxylic acid