VEIN BATCH 2027

النادي الطبي

Sub: Organic :المادة

Lecture: 1 :المحاضرة

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Edited: :تعديل

Lewis Structures

It only deals with VE

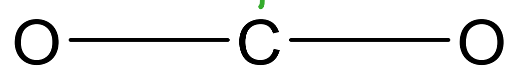
Lec 2

Procedure for obtaining good Lewis structures: eg. CO_2

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

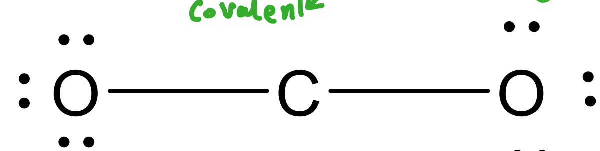
$$CO_2 = 4+2(6) = 16.$$

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.

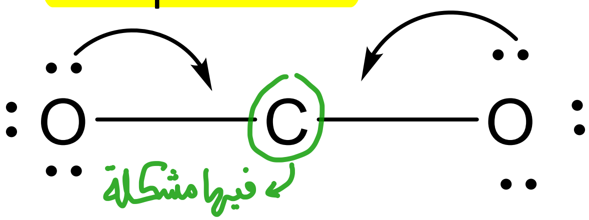


3) determine number of remaining e^-. complete the octet of the terminal atoms.

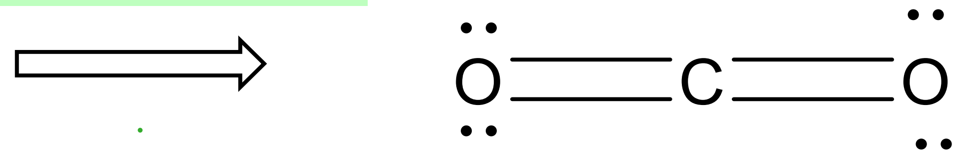
$$16 - 4 = 12$$



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



Check octet rule



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)

Formal charge = VE - (dashes + dots)

CO_2 → ماعليه شحنة إذاً لو حسبنا وجمعنا FC لازم تطلع صفر

For O 6-6 =0

For C 4-4 =0

$C = 4 - (4 + 0) = 0$ ✓✓

$O_1 = 6 - (2 + 4) = 0$ ✓✓

$O_2 = 6 - (2 + 4) = 0$ ✓✓

Ex: NO_3^- ← ION

* Formal Charge = ⊖1 → obtain an electron.

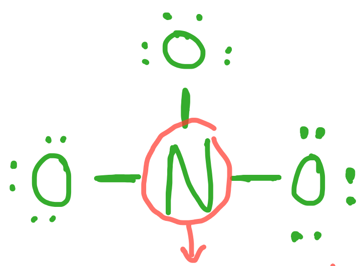
1. VE= 5+6*3+1 =24

N ↑ (5), O ↑ (6*3), كسب e^- ↑ (1)

2. Central atom → N

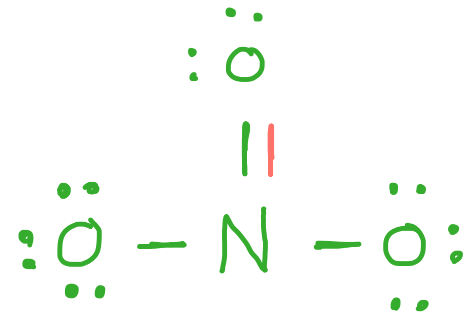
3. $24-6=18$

$18 \div 3 = 6$



incomplete octet

check → 4.



5. Formal charges → −1 لازم تطلع

1) $N = 5-(0+4) = +1$

2) $O_1 = 6-(1+6) = -1$

3) $O_2 = -1$

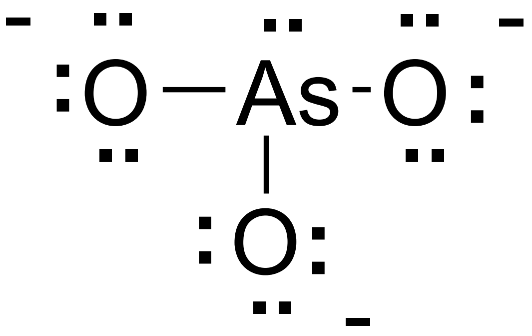
4) $O_3 = 6-(2+4) = 0$

مج $= +1 -1 -1 +0 = -1$ ✓✓

Lewis Structures (other examples)

Example 2: AsO_3^{3-}

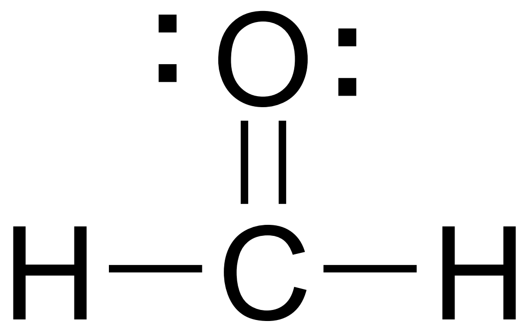
1) # e^-: 5 + 3(6) + 3 = 26
2) form 3 single bonds
3) 20 e^- remain
4) O needs 6, As needs 2
5) All octets
6) Formal charges



Lewis Structures (cont'd)

Example 3: CH_2O

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 = zero



Lewis Structures (cont'd)

Example 4: CO

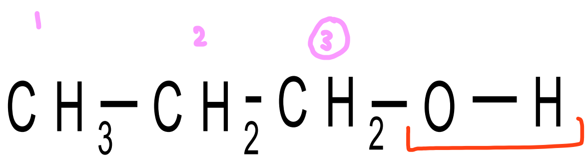
1) # e^-: 4 + 6 = 10
2) try 1 single bond
3) 8 e^- remain
4) C needs 6 as does O short 4 e^-
5) Share 4 more e^- - triple bond
6) Octets
7) Formal charges = zero

$$\overset{-1}{:C}\equiv\overset{+1}{O:}$$

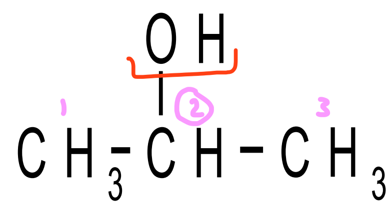
1.8 Isomers

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)

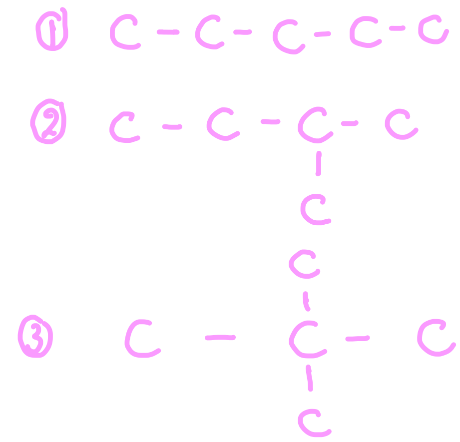


2-propanol
(bp 82.4 C)

1.9 Writing Structural Formulas

تطابق وتوافق

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

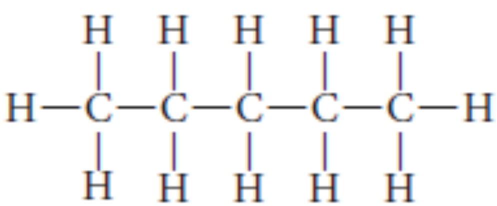


C - C - C -C - C

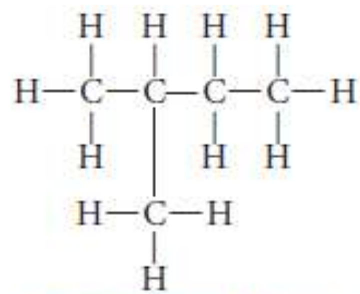
Continuous chain (unbranched)

C - C -C – C
C

Branched chain



pentane, bp 36°C



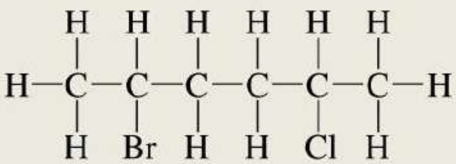
2-methylbutane, bp 28°C
(isopentane)

C forms 4 covalent bonds

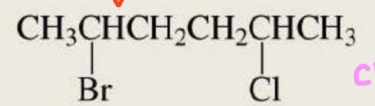
Dash formula

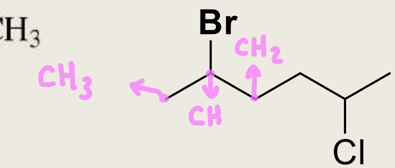
Kekulé structure	Condensed structures	Bond line formula

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

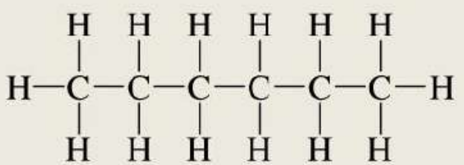


$CH_3CHBrCH_2CH_2CHClCH_3$ or



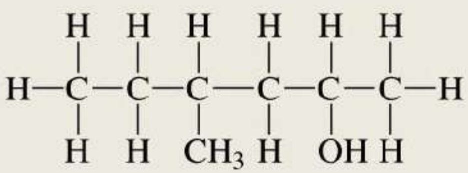


Repeating CH_2 groups can be shown in parentheses. (أقواس)

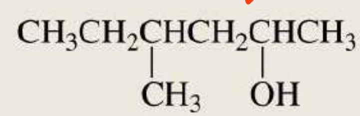


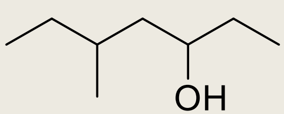
$CH_3CH_2CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_4CH_3$

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

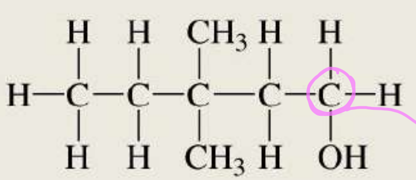


$CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$ or

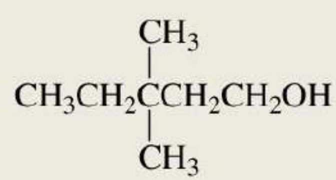


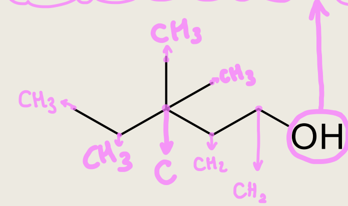


Groups bonded to the far-right carbon are not put in parentheses.



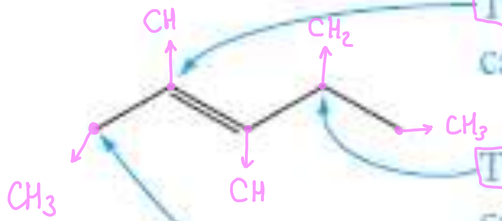
$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or





ما بنظهر ال bonds

$CH_3CH{=}CHCH_2CH_3$

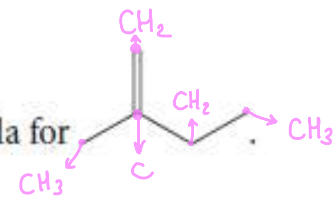


Three line segments emanate from this point; therefore, this carbon has one hydrogen $(4 - 3 = 1)$ attached to it.

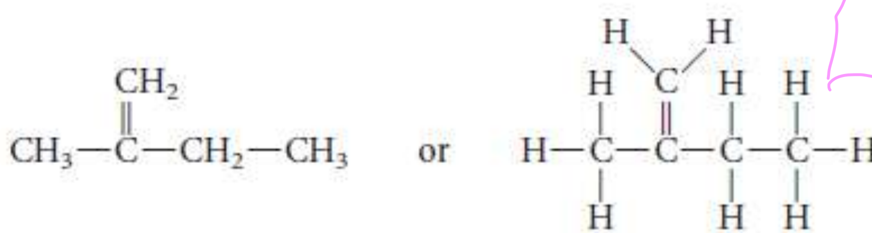
Two line segments emanate from this point; therefore, this carbon has two hydrogens $(4 - 2 = 2)$ attached to it.

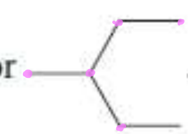
One line segment emanates from this point; therefore, this carbon has three hydrogens $(4 - 1 = 3)$ attached to it.

EXAMPLE 1.12

Write a more detailed structural formula for  .

Solution



PROBLEM 1.23 Write a more detailed structural formula for 

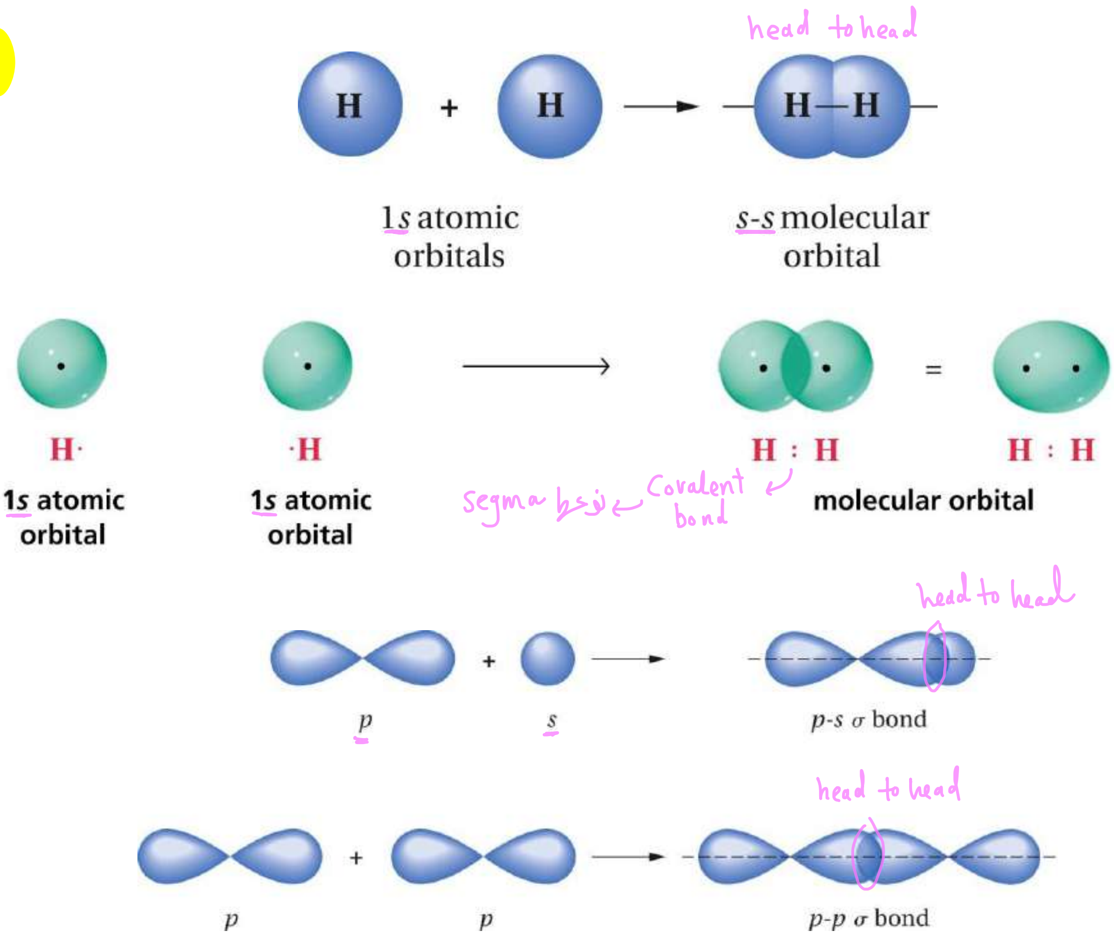
$CH_3-O-CH_2-CH_3$ جواب

* موكل نقطة Carbon

$\rightarrow$ $CH_3-CH(CH_2CH_3)-CH_2CH_3$ (or)

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.



* تداخل بالأفلاك حقيقي ومباشر (أقوى)

* ممكن مثلاً تداخل فلك S مع S أو
P مع S أو
P مع P ..... الخ

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

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

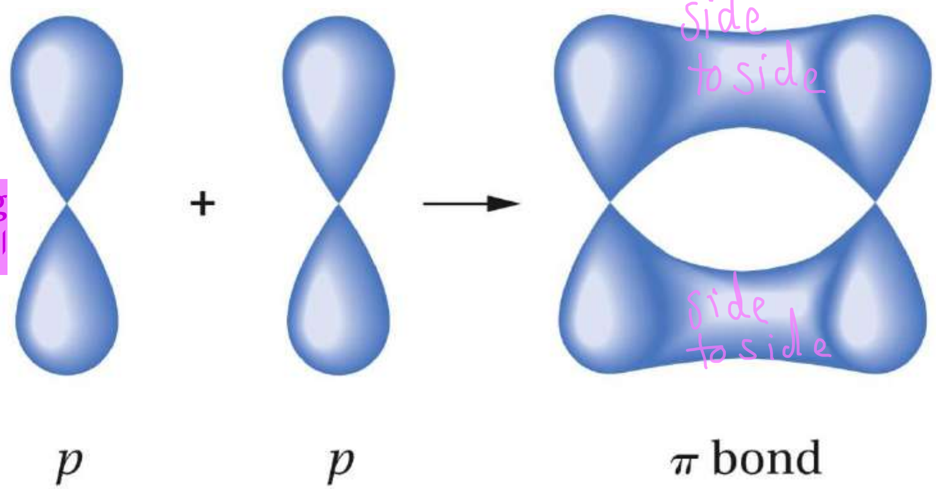
شروط:
1. 2 P orbitals.
2. parallel.

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.

π bonds are formed by the ① **side to side overlap** of ② 2 "p" orbitals only

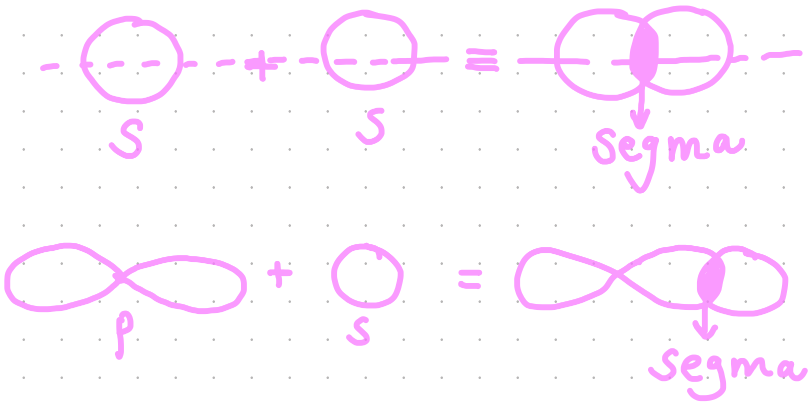
تداخل غير مباشر

There is no real overlabing (side to side) التداخل بكون

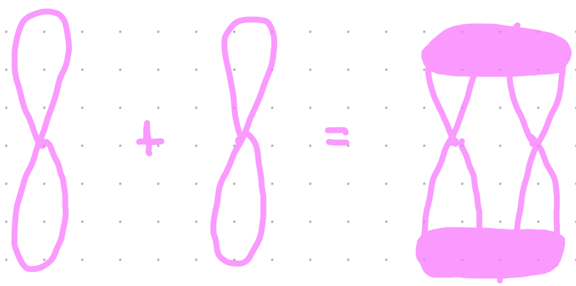


Segma bond	Pi bond
along the internuclear axis	Isn’t located along the internuclear axis But on the side of the axis
Real overlabing تداخل حقيقي و مباشر	Isn’t a real overlabing تداخل غير مباشر
Formed by head to head fashion	Formed by side to side overlap
Stronger	2 (p) parallel orbitals

Ex



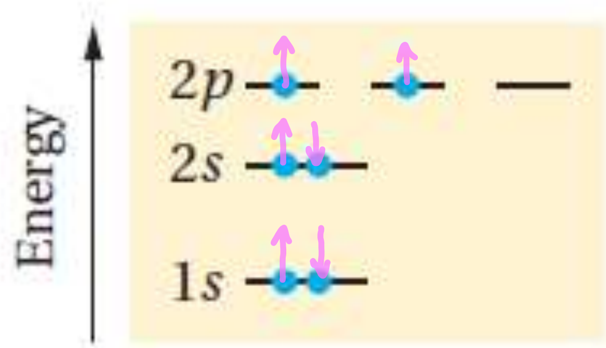
Ex:



Carbon sp^3 Hybrid Orbitals

مهجن

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

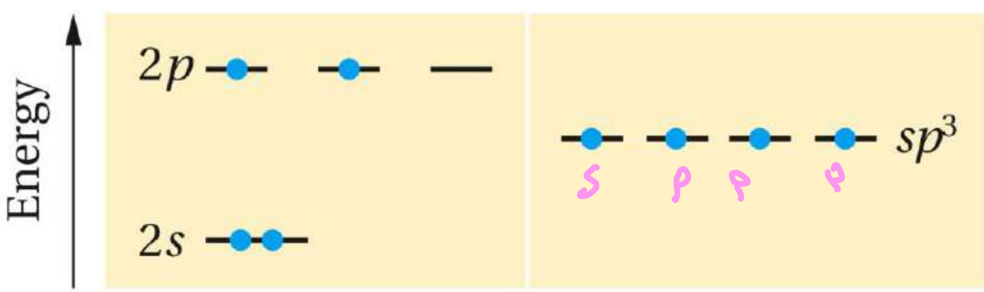


Distribution of the six electrons in a carbon atom. Each dot stands for an electron. according to energy.

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

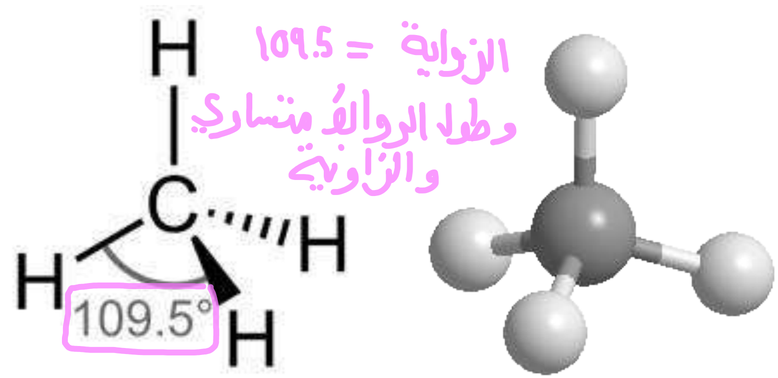
A: We know from experience that carbon usually forms *four* single bonds, and often these bonds are all equivalent, as in CH_4

الشرح

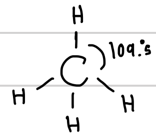


Atomic orbitals of carbon

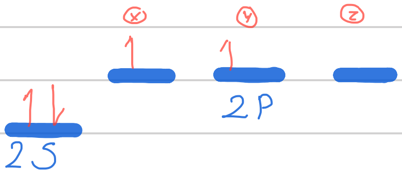
Four equivalent sp^3 hybrid orbitals



3D Structure of Methane Molecule

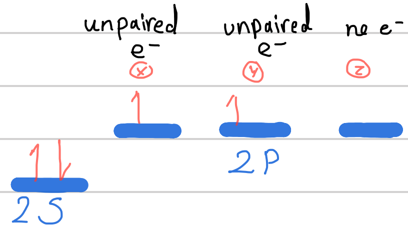
* CH_4 ←  الزواية و الطول متساوي بين كل رابطة ورابطة بين C و H .

* توزيع (C) : $1S^2, 2S^2, 2P^2$
lower energy ←
و e^- ترتيب حسب energy



رسمة valence electron

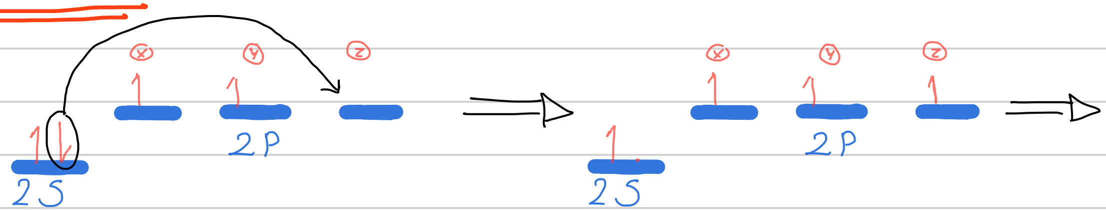
* اذا بدي أجيب 4 H و كل واحد فيهم عنده الكترون



من هون اجت قصة Hybirdization ، لتوضح سبب تكوين الكربون لأربع روابط

وهي بتتضمن 2steps :

① Promotion from 2S to 2P.

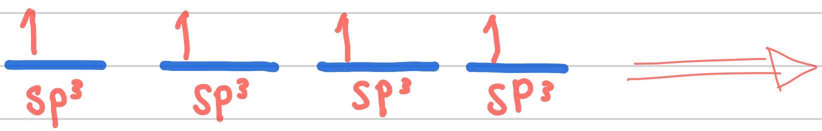


الآن أصبحت الكربونة قادرة انها تعمل أربع روابط لكن

لو أمعنا النظر بنشوف انه 3 منهم الهم شكل وطاقة متساوية وواحد منهم اله شكل وطاقة مختلفة والي هو (S)

② Hybridization : وهون اجيب 2S واخلطها مع ال 2P

والناتج 4 orbitals كل واحد اسمه Sp^3 .

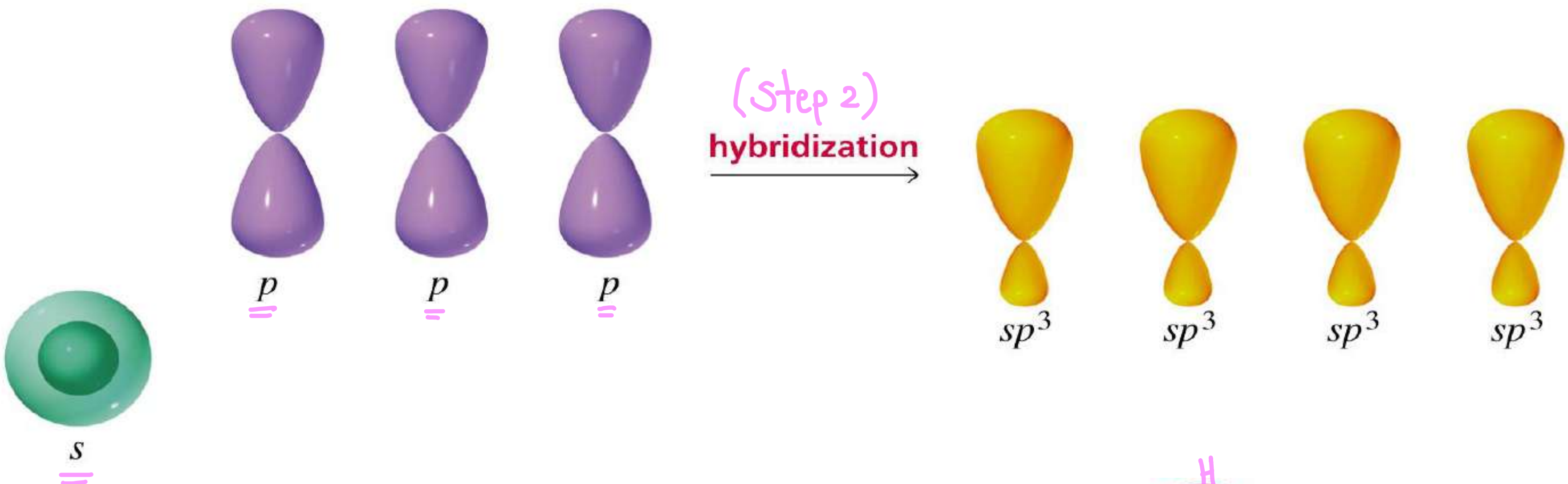


متساويات في الطاقة والشكل

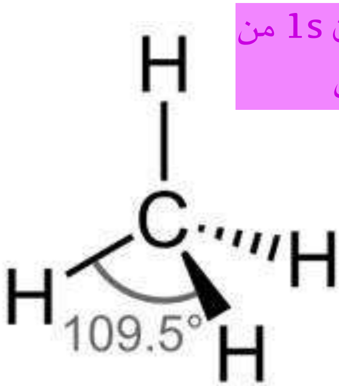
فلما عملت segma مع كل وحدة راح يكون ال4 covalent bond نفس الطول والزاوية

وهاي هي الظاهرة الي فسرت الي ليش (C) بكون 4 روابط متساويات ① بالطول و ② الزاوية و ③ الشكل و ④ الطاقة

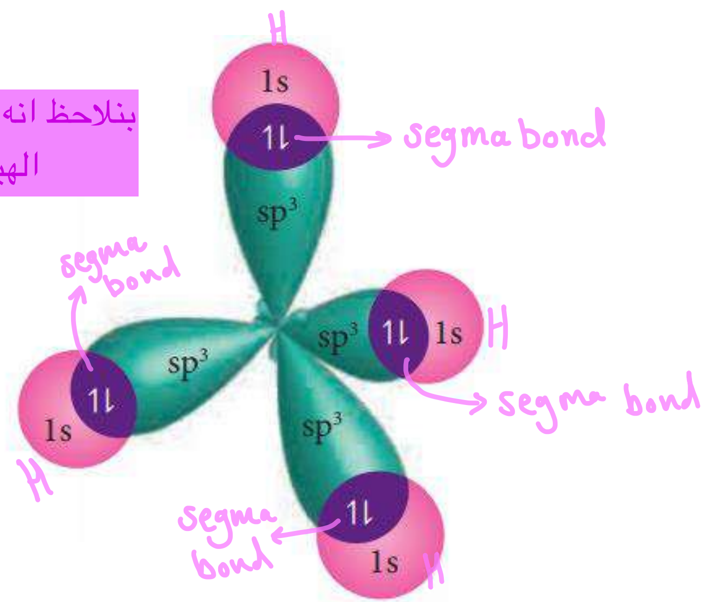
Mix or combine the four atomic orbitals of the valence shell to form four identical hybrid orbitals



tetrahedral

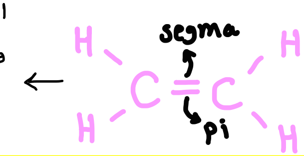


بنلاحظ انه sigma bond حصلت بين 1s من الهيدروجين و sp3 من الكربون



SP^2-Hybridized orbitals

الكربونة الوحدة تتكون من SP^3 ، لحتى نعمل رابطة Pi نحنا بحاجة لـ P من كل كربونة
فبضل للـ segma SP^2 ، حنخلط ونعمل Hybridization كالتالي :

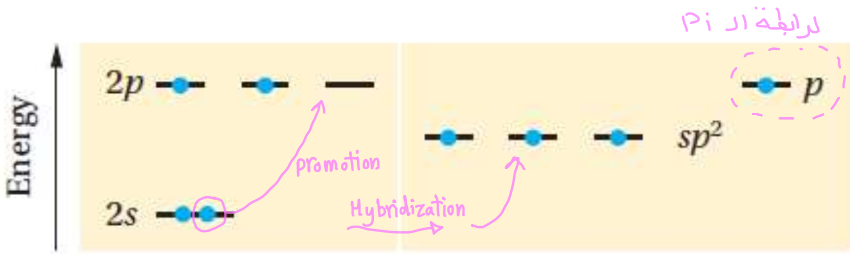


2s 2p 2p 2p → sp² sp² sp² Px

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

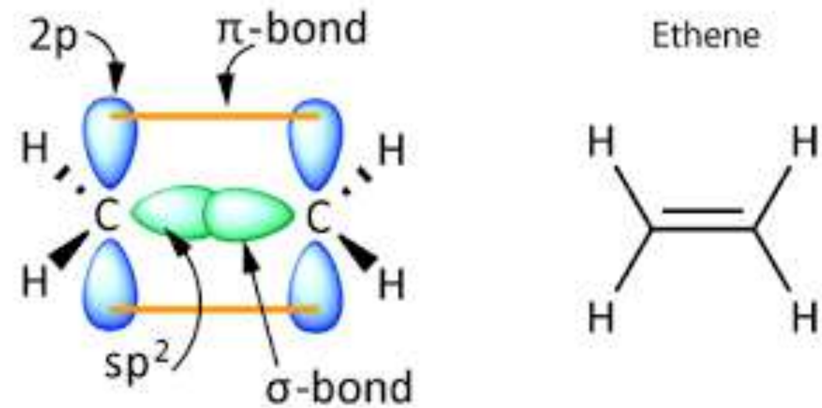
ذروة وقمة

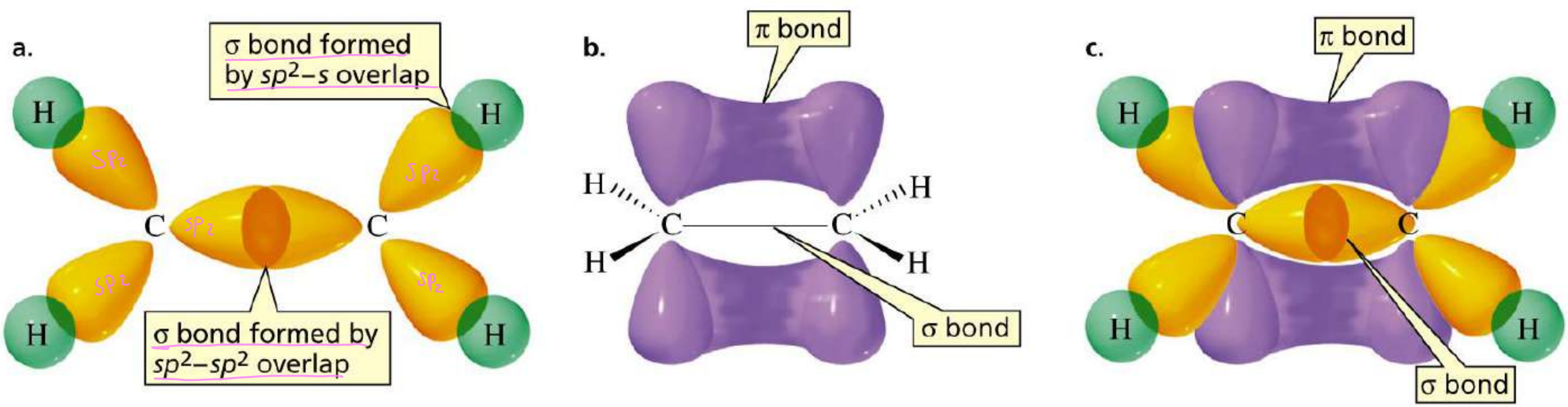
Trigonal planer



Atomic orbitals of carbon

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



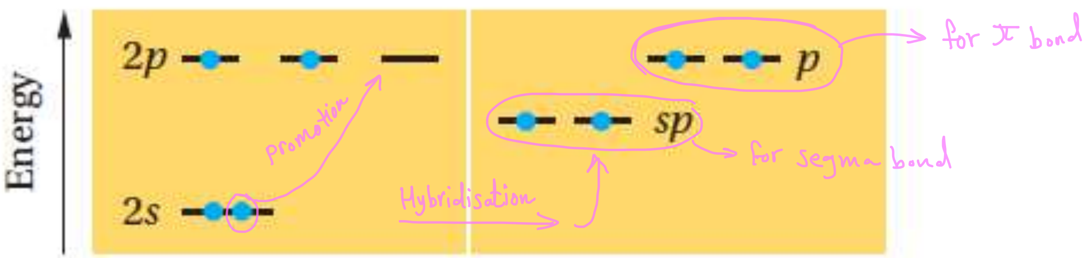


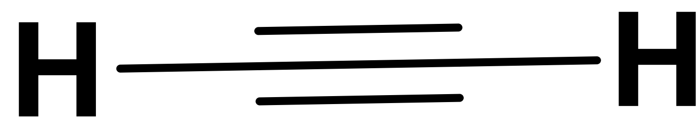
SP-Hybridized orbitals

Bonding in Ethyne: **A Triple Bond**

$H-C\equiv C-H$

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

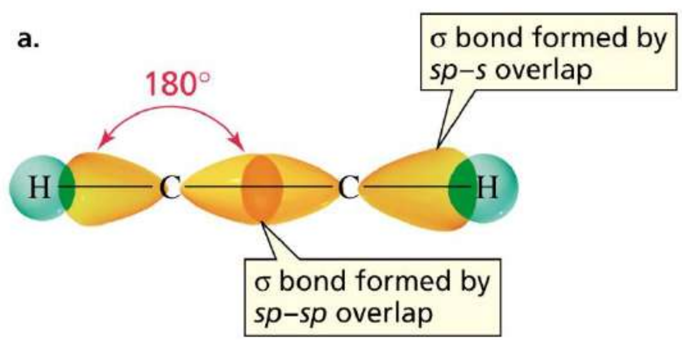


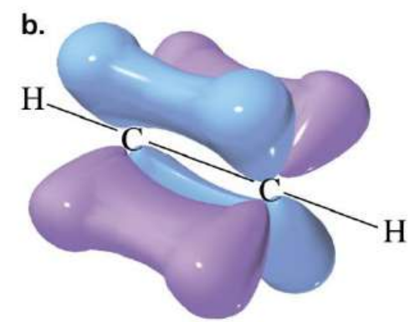


Atomic orbitals of carbon

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





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°	linear
1, 2	3 sp^2	120°	trigonal planar
1, 3	4 sp^3	109°	tetrahedral

https://youtu.be/gfrxRGQeimw ← شرحي لِ hybridization

New terms from the second lecture

* Obtain : get
* Terminal : طرفي
* central : مركزي
*correspond : تطابق و توافق
* parentheses : أقواس
* emanate : تنبعث
* density : كثافة
* axis : محاور
* hybrid : هجين

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.

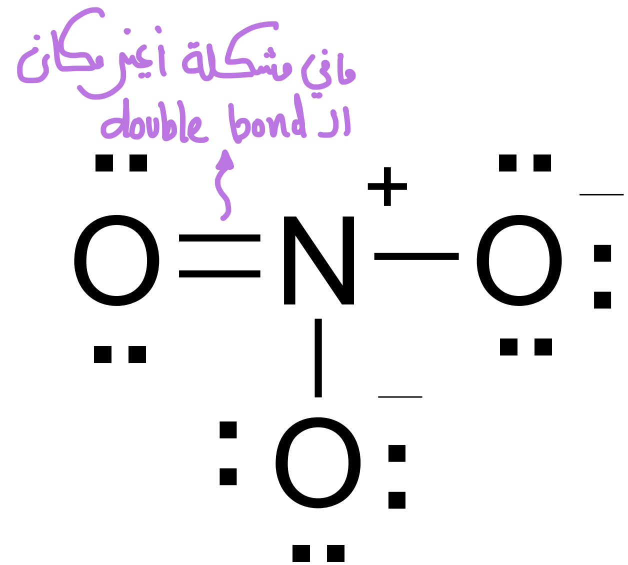
The assumption in these diagrams is that the atom positions do not change, we are only allowed to change the distribution of e^-, *i.e.* the bonds and lone pairs.

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

لا تشرح هياكل لويس دائمًا خصائص الجزيئات. نظرية الرنين هي نهج الطبقات الثانية.

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)

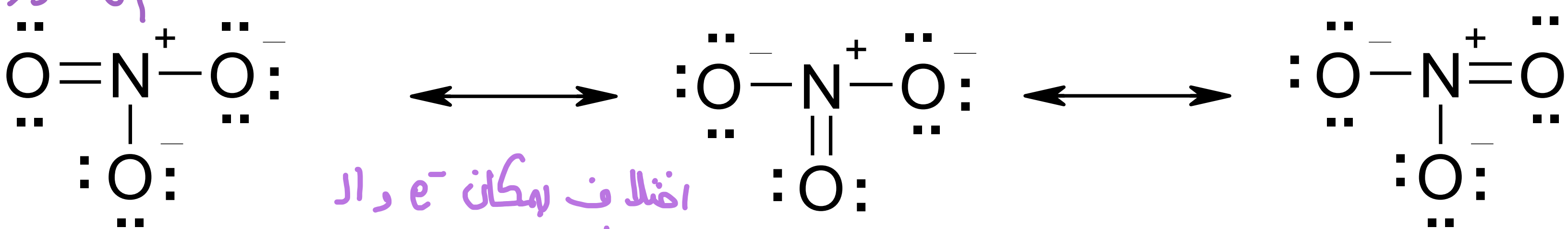
Example 1: NO_3^- (cont'd)

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 the oxygen.

وبال 3 حالات عنا correct Lewis structure

عن طريق نفد segma

sp²



اختلاف في مكان e^- وال double bonds

↳ resonance

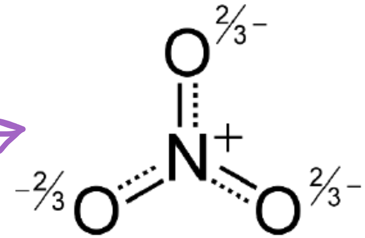
Electrons aren't localized, they are delocalized

A B C

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

وبالحقيقة هاد هو شكل المركب بالحقيقة ، هي لا single ولا double بتوخد ال characteristic تبعت ال single double

ال e^- عم تنتقل من مكان الى مكان (Resonance)



A resonance hybrid

Resonance : مركب اله أكثر من شكل ، الاختلاف بينهم بكون بتوزيع e^- أو مكان الـ double or triple.

ويمنع فيها تغيير مكان أي atom.

شروط : ١. الالكترونات تكون ← lone pair ..
← = ≡ ← π bond ، – ممنوع segma

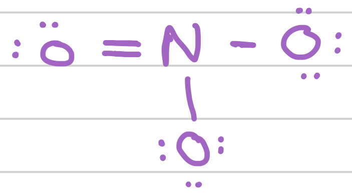
(طبعا قصدنا الذرات الطرفية)

٢. نوع التهجين ← SP / SP^2

طيب كيف نعرف؟ عن طريق عدد الـ segma ، فلو كان عنا 3 سيغما بكون SP^2
لو عنا 2 سيغما بكون SP

(طبعا بكون الـ atom اللي بالنص)

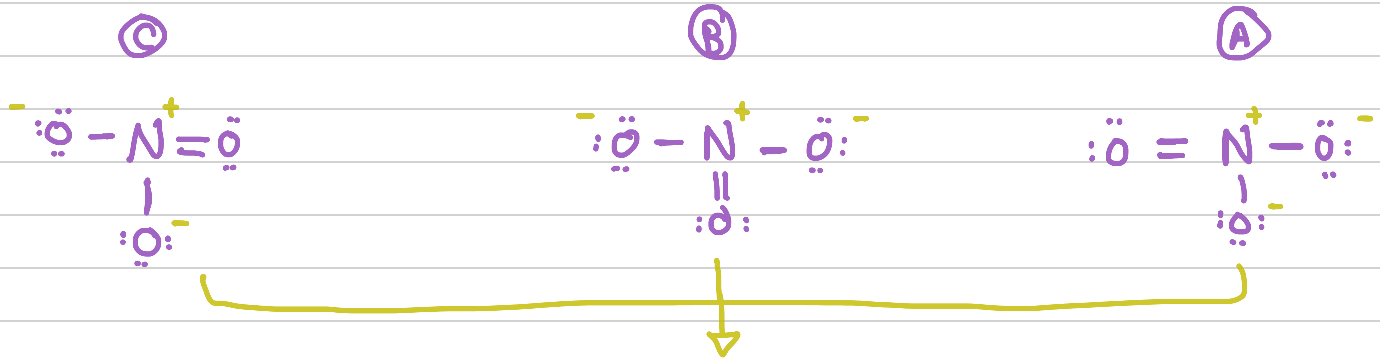
أمثلة : NO_3^- ← الرسم :



، هل الـ شرط resonance ؟ الجواب نعم

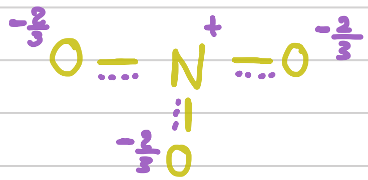
① عنا التهجين SP^2

② الالكترونات = lone pair و



إذا الـ ١٣ أشكال تختلف عن بعضها بـ double bond و single bond

Hybrid between (A,B,C) وشكله الحقيقي بكون



والسبب الحقيقي انه الـ double موجودة بالثلاث أماكن بنفس الوقت أو ينتقل من مكان لمكان ← بنسميه resonance والذي ينتقل الالكترونات الـ π

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

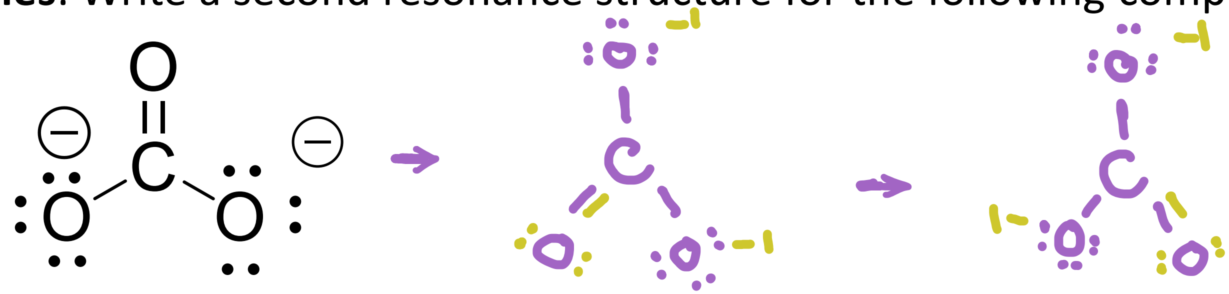
شرطين لأقدر ارسم Resonance

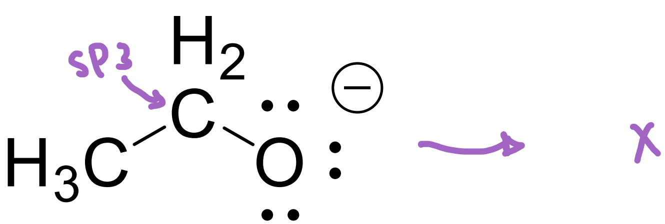
Rules for drawing resonance structures :

1) Electrons only can be ~~oved~~ moved (lone pair / π electrons) , but not segma.

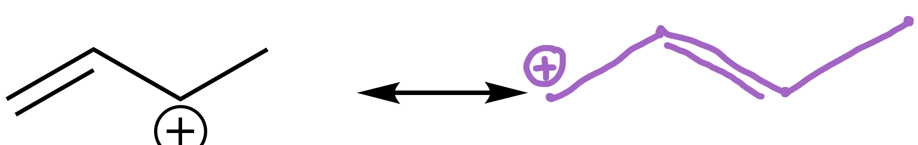
2) Electrons move toward SP/ SP^2 hybridized atom only, but not SP^3 → لأنه ما عنده باي يستقبل الالكترونات

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



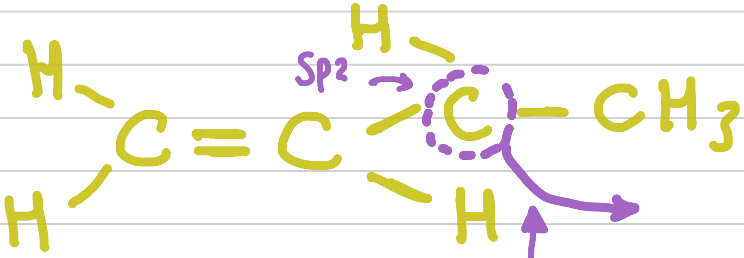


Exercise



other example: $CH_3 - \ddot{O}:$

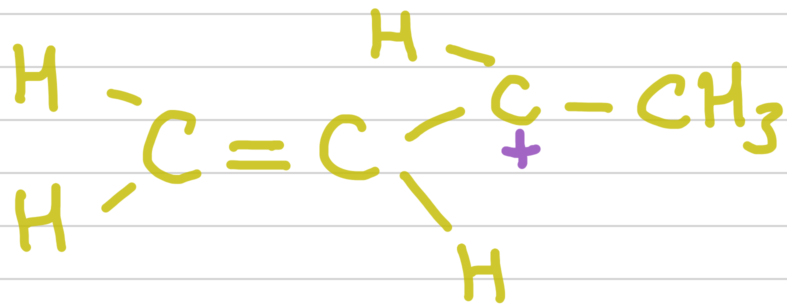
① الشروط :- 1 ✓ 2 ✗ ← لأنه SP_3 ، الكربون ما في مجال تستقبل الالكترونات .



* نوع Hybridization : Sp^2 ،

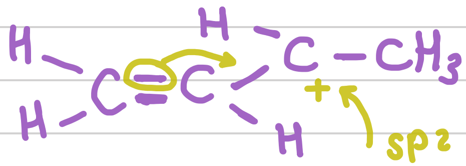
عشان هاي الرابطة ناقصة
↓
Charged
↓
Positively charged
↓
بنحسب من formed charge

$$[VE-(dot+dash)]$$
$$4-(0+3)=+1$$



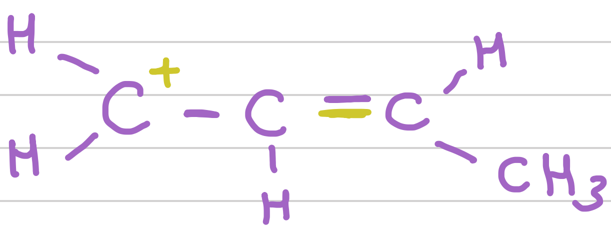
* طيب كيف بنرسم Resonance ؟

1. بنيجي عالكربونتين الي بينهم π وبنعمل push ونقل لـ double bond باتجاه الكربونة الي هي SP_2



2. انتقلت الرابطة ← غيرت مكان الالكترونات وحركنا π electron ،

اذا بقدر احكي عنه Resonance



NOTE:

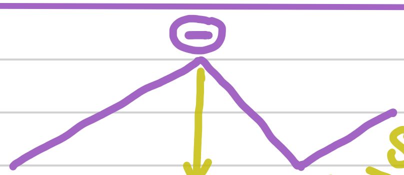
sp^3

sp_2

يقدر أعمل الـ Pushing

غير مسموح أعمل هيك

مسموح أمشي هيك



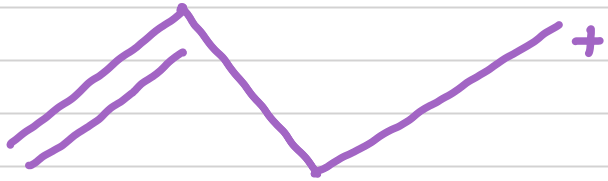
بصير هون انتقال لو

كان عنا هون sp^2 or sp

يعني جنبها sp أو sp^2

هون فرضاً جنبها ماي sp أو sp^2 لذا ممنوع يصير انتقال

سؤال ؟؟



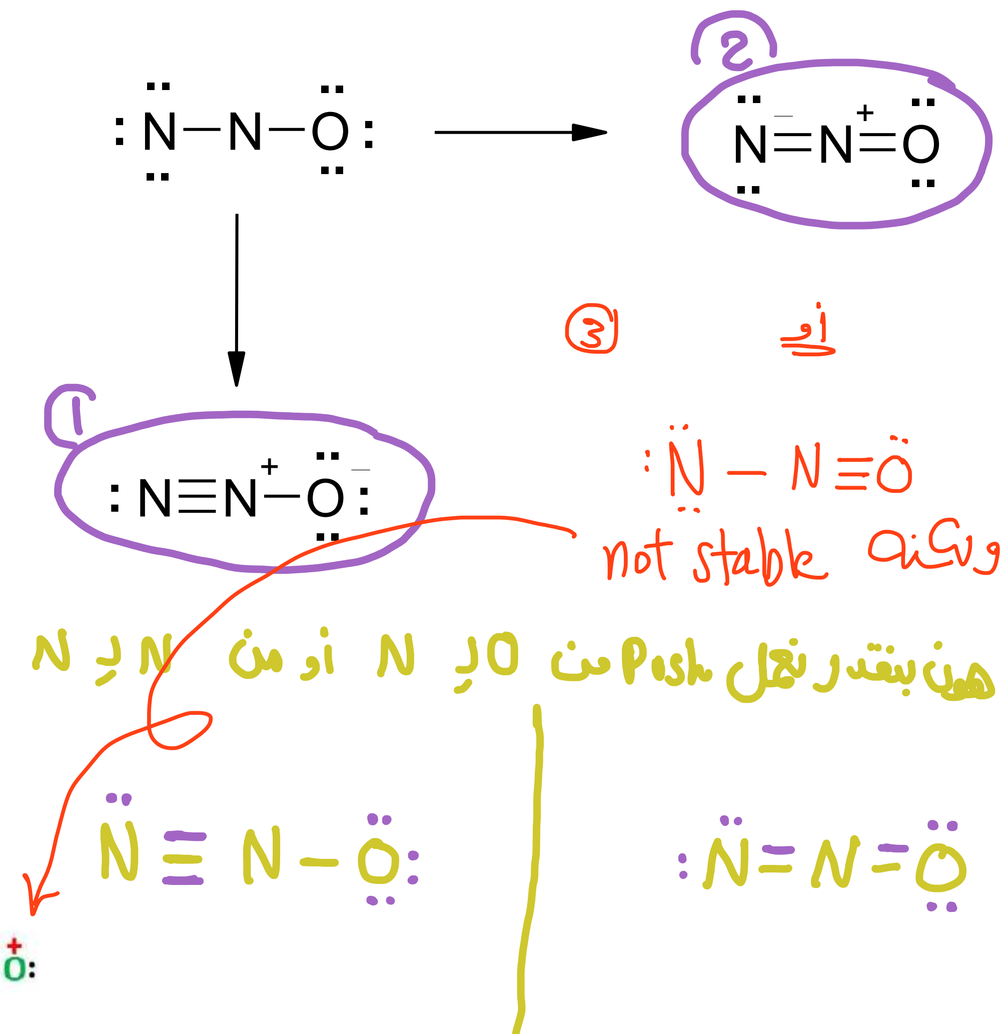
هل لهذا المركب يوجد resonance؟

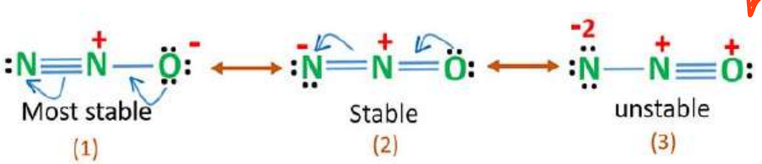
لا، صحيح في عنا double bond و sp_2 ولكنهم مو direct وبعيدين عن بعض

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?



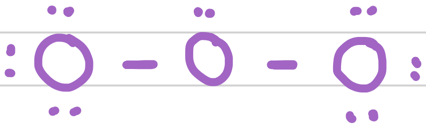


أسئلة إضافية من عندي ، جربوا حلوهم (:

① O_3 :

$\#e^- = 6 \times 3 = 18$

نوع التهجين؟؟

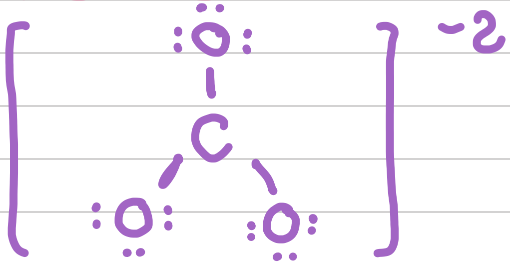


الشروط :- 1 ✓ 2 ✓

الرسم :

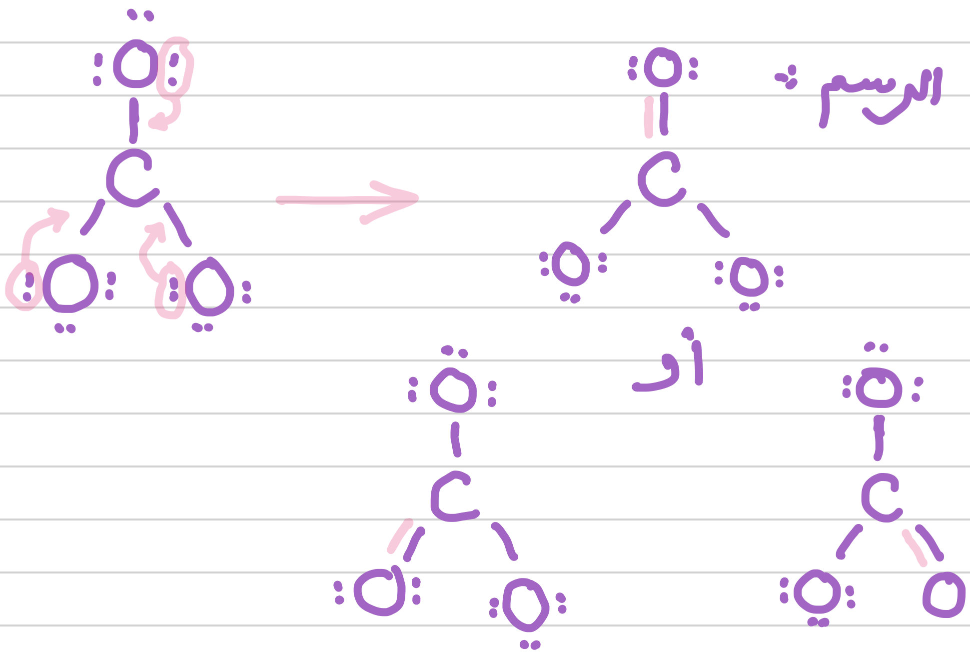
② CO_3^{-2} :

$4 + (6 \times 3) + 2 = 24$



الشروط : 1 ✓ 2 ✓

الرسم :



1.17: Classification According to Molecular Framework

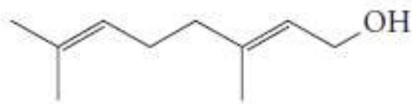
- The three main classes of molecular frameworks for organic structures are **acyclic**, **carbocyclic**, and **heterocyclic** compounds.

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

بتكون مفتوحة

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

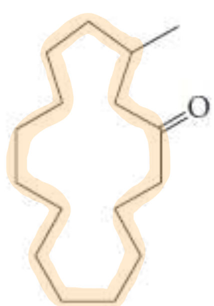
$CH_3C(=O)(CH_2)_4CH_3$

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

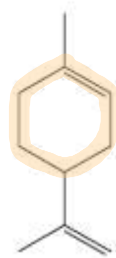
1.17b: Carbocyclic Compounds: contain rings of carbon atoms

حلقية و المكون تبعها carbon

← هدولا الحلقات كلهم كربونات



muscone
(musk deer)
bp 327–330°C

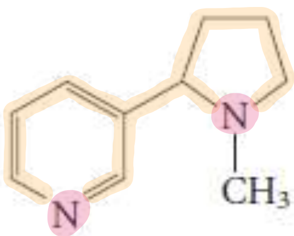


limonene
(citrus fruit oils)
bp 178°C

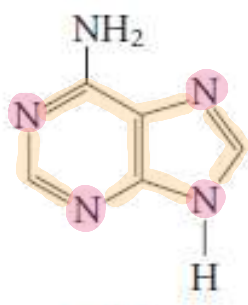
benzene
(petroleum)
mp 5.5°C, bp 80.1°C

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...)

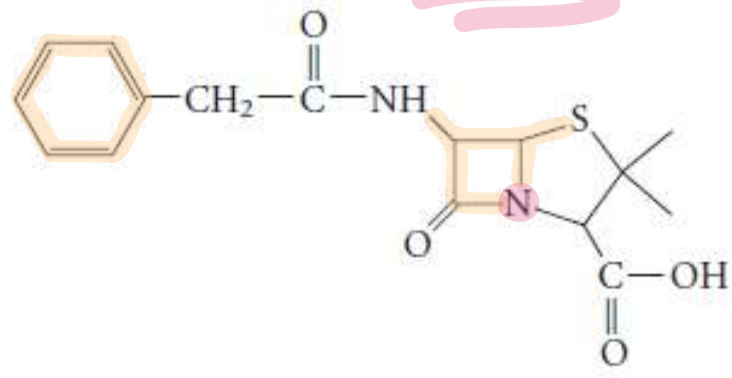
SON



nicotine
bp 246°C



adenine
mp 360–365°C
(decomposes)



penicillin-G
(amorphous solid)

تم استبدال ذرة أو أكثر من ذرة كربون بـ (SON)

احفظوهم عالترتيب

الابن = Son

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

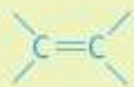
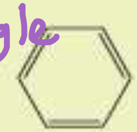
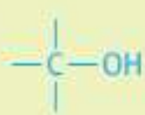
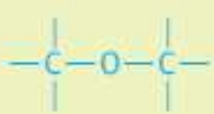
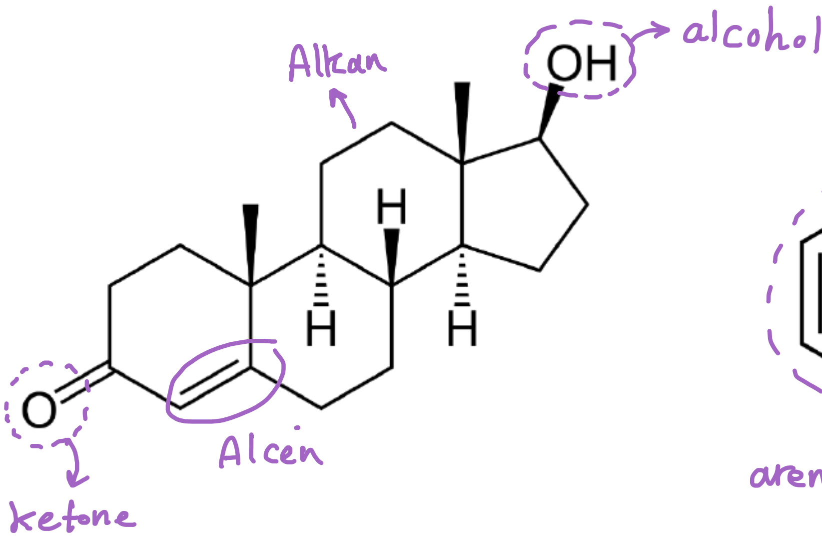
	Structure	Class of compound	Specific example	Common name of the specific example
A. Functional groups that are a part of the molecular framework		alkane	$CH_3—CH_3$	ethane, a component of natural gas
		alkene	$CH_2═CH_2$	ethylene, used to make polyethylene
	—C≡C—	alkyne	HC≡CH	acetylene, used in welding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

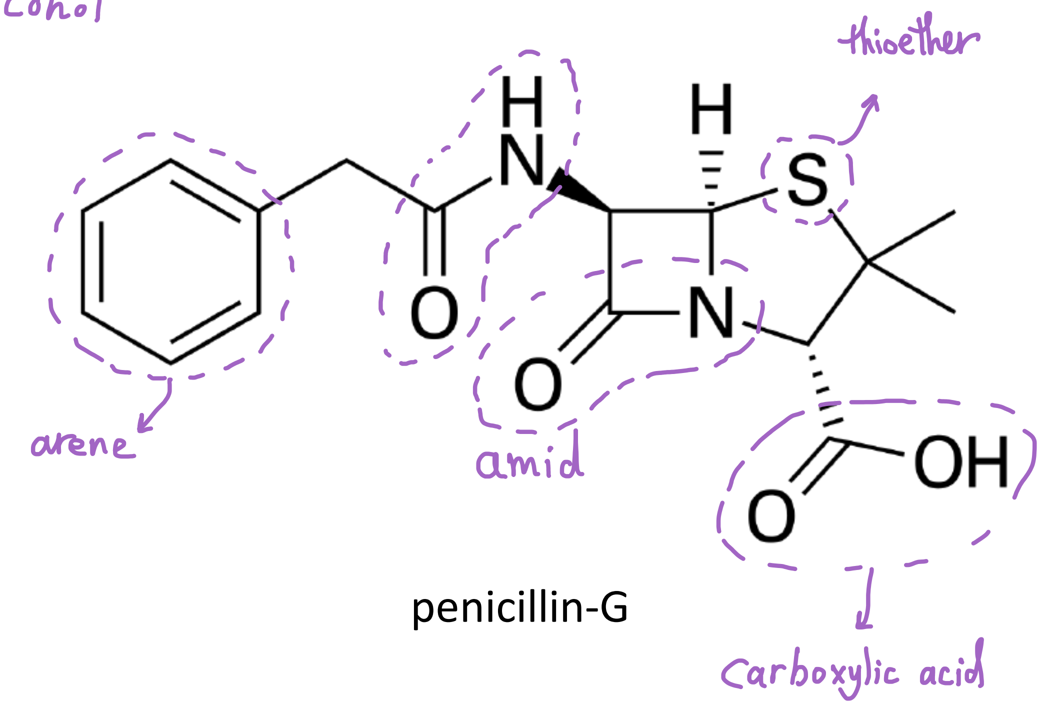
Table 1.6 continued

	Structure	Class of compound	Specific example	Common name of the specific example
*2. With carbon–oxygen double bonds**	$-C(=O)-H$	aldehyde	$CH_2{=}O$	formaldehyde, used to preserve biological specimens
	$-\overset{\vert}{\underset{\vert}{C}}-C(=O)-\overset{\vert}{\underset{\vert}{C}}-$	ketone	$CH_3C(=O)CH_3$	acetone, a solvent for varnish and rubber cement
3. With single and double carbon–oxygen bonds	$-C(=O)-OH$	carboxylic acid	$CH_3C(=O)-OH$	acetic acid, a component of vinegar
	$-C(=O)-O-\overset{\vert}{\underset{\vert}{C}}-$	ester	$CH_3C(=O)-OCH_2CH_3$	ethyl acetate, a solvent for nail polish and model airplane glue
*C. Functional groups containing nitrogen***	$-\overset{\vert}{\underset{\vert}{C}}-NH_2$	primary amine	$CH_3CH_2NH_2$	ethylamine, smells like ammonia
	$-C{\equiv}N$	nitrile	$CH_2{=}CH-C{\equiv}N$	acrylonitrile, raw material for making Orlon
D. Functional group with oxygen and nitrogen	$-C(=O)-NH_2$	primary amide	$H-C(=O)-NH_2$	formamide, a softener for paper
E. Functional group with halogen	$-X$	alkyl or aryl halide	CH_3Cl	methyl chloride, refrigerant and local anesthetic
F. Functional groups containing sulfur†	$-\overset{\vert}{\underset{\vert}{C}}-SH$	thiol (also called mercaptan)	CH_3SH	methanethiol, has the odor of rotten cabbage
	$-\overset{\vert}{\underset{\vert}{C}}-S-\overset{\vert}{\underset{\vert}{C}}-$	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?



testosterone



penicillin-G

Classification of organic compounds

According to

- molecular framework
  - acyclic → مفتوحة
  - Carbocyclic → حلقة من الكربونات
  - heterocyclic → حلقة وتم استبدال الكربون بذرة اخرى مثل (SON)
- Functional

New vocabulary

Assumption: افتراض

Distinctive: مميز

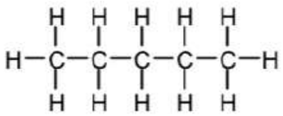
Resonance: مركب اله اكتر من (structure) بيختلفوا عن بعض بتوزيع الالكترونات

Chapter Summary*

An **atom** consists of a nucleus surrounded by **electrons** arranged in **orbitals**. The electrons in the outer shell, or the **valence electrons**, are involved in bonding. **Ionic bonds** are formed by electron transfer from an **electropositive** atom to an **electronegative** atom. Atoms with similar electronegativities form **covalent bonds** by sharing electrons. A **single bond** is the sharing of one electron pair between two atoms. A covalent bond has specific **bond length** and **bond energy**.

Carbon, with four valence electrons, mainly forms covalent bonds. It usually forms four such bonds, and these may be with itself or with other atoms such as hydrogen, oxygen, nitrogen, chlorine, and sulfur. In pure covalent bonds, electrons are shared equally, but in **polar covalent bonds**, the electrons are displaced toward the more electronegative element. **Multiple bonds** consist of two or three electron pairs shared between atoms.

Structural (or **constitutional**) **isomers** are compounds with the same **molecular formulas** but different **structural formulas** (that is, different arrangements of the atoms in the molecule). **Isomerism** is especially important in organic chemistry because of the capacity of carbon atoms to be arranged in so many different ways: continuous chains, branched chains, and rings. Structural formulas can be written so that every bond is shown, or in various abbreviated forms. For example, the formula for *n*-pentane (*n* stands for normal) can be written as:

 or $CH_3CH_2CH_2CH_2CH_3$ or 

Some atoms, even in covalent compounds, carry a **formal charge**, defined as the number of valence electrons in the neutral atom minus the sum of the number of unshared electrons and half the number of shared electrons. **Resonance** occurs when we can write two or more structures for a molecule or ion with the same arrangement of atoms but different arrangements of the electrons. The correct structure of the molecule or ion is a **resonance hybrid** of the **contributing structures**, which are drawn with a double-headed arrow (↔) between them. Organic chemists use a curved arrow (↷) to show the movement of an electron pair.

A **sigma** (σ) **bond** is formed between atoms by the overlap of two atomic orbitals along the line that connects the atoms. Carbon uses ***sp*³-hybridized orbitals** to form four such bonds. These bonds are directed from the carbon nucleus toward the corners of a tetrahedron. In **methane**, for example, the carbon is at the center and the four hydrogens are at the corners of a regular tetrahedron with H–C–H bond angles of 109.5°.

Carbon compounds can be classified according to their molecular framework as **acyclic** (*not* cyclic), **carbocyclic** (containing rings of carbon atoms), or **heterocyclic** (containing at least one ring atom that is not carbon). They may also be classified according to **functional group** (Table 1.6).

Summary من الكتاب

سؤال عالتشابتر من الكتاب ت

Ch1 3. How many σ (sigma) bonds are there in CH_2=CH–CH=CH_2?
1. 3 2. 9 3. 10 4. 11 5. 12