

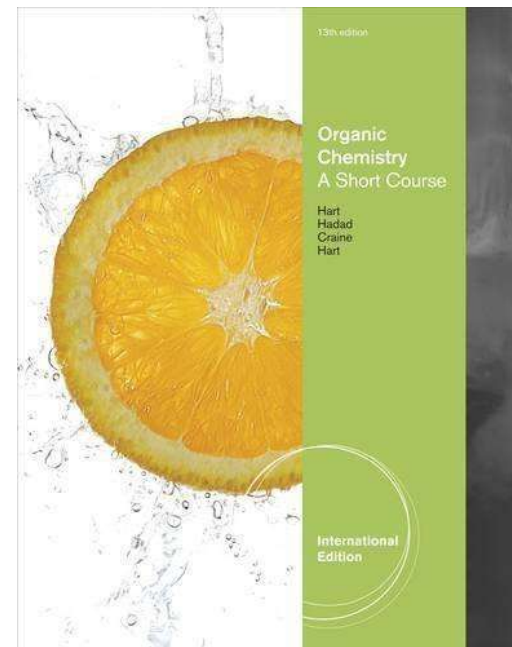
Chem 237 Basics of Organic Medicinal Chemistry

- **Course description**

This is the first year organic chemistry course, introducing basic concepts and principles of organic chemistry (chapters 1 – 11).

- **Texts**

Hart, Craine, Hart and Hadad, Organic Chemistry, A Short Course, 13th Edition (Brooks/Cole, Cengage Learning, CA 94002-3098 USA, 2012).



Periodic Table of the Elements

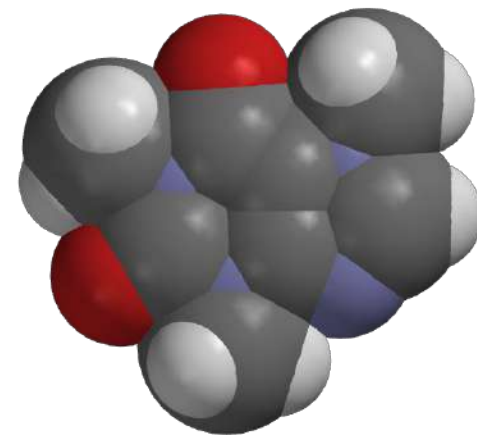
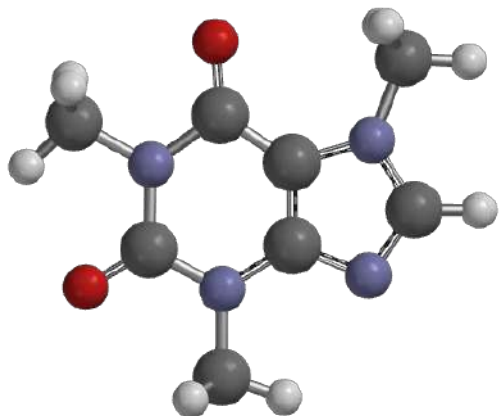
1 IA H Hydrogen 1.008 1	2 IIA He Helium 4.0026 2											13 IIIA B Boron 10.81 2-3	14 IVA C Carbon 12.011 2-4	15 VA N Nitrogen 14.007 2-5	16 VIA O Oxygen 15.999 2-6	17 VIIA F Fluorine 18.998 2-7	18 VIIIA Ne Neon 20.180 2-8
3 Li Lithium 6.94 2-1	4 Be Beryllium 9.012 2-2											13 Al Aluminium 26.982 2-8-3	14 Si Silicon 28.085 2-8-4	15 P Phosphorus 30.974 2-8-5	16 S Sulfur 32.06 2-8-6	17 Cl Chlorine 35.45 2-8-7	18 Ar Argon 39.948 2-8-8
11 Na Sodium 22.98976928 2-8-1	12 Mg Magnesium 24.305 2-8-2	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 Ga Gallium 69.723 2-8-13	14 Ge Germanium 72.630 2-8-14	15 As Arsenic 74.922 2-8-15	16 Se Selenium 78.971 2-8-16	17 Br Bromine 79.904 2-8-17	18 Kr Krypton 83.798 2-8-18
19 K Potassium 39.0983 2-8-9-1	20 Ca Calcium 40.078 2-8-9-2	21 Sc Scandium 44.955908 2-8-9-2	22 Ti Titanium 47.867 2-8-9-2	23 V Vanadium 50.9415 2-8-9-2	24 Cr Chromium 51.9961 2-8-9-2	25 Mn Manganese 54.938044 2-8-9-2	26 Fe Iron 55.845 2-8-9-2	27 Co Cobalt 58.933 2-8-9-2	28 Ni Nickel 58.693 2-8-9-2	29 Cu Copper 63.546 2-8-9-2	30 Zn Zinc 65.38 2-8-9-2	31 In Indium 114.82 2-8-18-3	32 Sn Tin 118.71 2-8-18-4	33 Sb Antimony 121.76 2-8-18-5	34 Te Tellurium 127.60 2-8-18-6	35 Br Bromine 79.904 2-8-17	36 Kr Krypton 83.798 2-8-18
37 Rb Rubidium 85.4678 2-8-18-1	38 Sr Strontium 87.62 2-8-18-2	39 Y Yttrium 88.90584 2-8-9-2	40 Zr Zirconium 91.224 2-8-18-2	41 Nb Niobium 92.90637 2-8-18-2	42 Mo Molybdenum 95.94 2-8-18-2	43 Tc Technetium 98.00 2-8-18-2	44 Ru Ruthenium 101.07 2-8-18-2	45 Rh Rhodium 102.91 2-8-18-2	46 Pd Palladium 106.42 2-8-18-2	47 Ag Silver 107.87 2-8-18-2	48 Cd Cadmium 112.41 2-8-18-2	49 In Indium 114.82 2-8-18-3	50 Sn Tin 118.71 2-8-18-4	51 Sb Antimony 121.76 2-8-18-5	52 Te Tellurium 127.60 2-8-18-6	53 I Iodine 126.90 2-8-18-7	54 Xe Xenon 131.29 2-8-18-8
55 Cs Cesium 132.90545196 2-8-18-8-1	56 Ba Barium 137.327 2-8-18-8-2	57-71 Lanthanides	72 Hf Hafnium 178.49 2-8-18-32-2	73 Ta Tantalum 180.94788 2-8-18-32-2	74 W Tungsten 183.84 2-8-18-32-2	75 Re Rhenium 186.21 2-8-18-32-2	76 Os Osmium 190.23 2-8-18-32-2	77 Ir Iridium 192.22 2-8-18-32-2	78 Pt Platinum 195.08 2-8-18-32-2	79 Au Gold 196.97 2-8-18-32-2	80 Hg Mercury 200.59 2-8-18-32-2	81 Tl Thallium 204.38 2-8-18-32-3	82 Pb Lead 207.2 2-8-18-32-4	83 Bi Bismuth 208.98 2-8-18-32-3	84 Po Polonium 209 2-8-18-32-4	85 At Astatine (210) 2-8-18-32-5	86 Rn Radon 222 2-8-18-32-8
87 Fr Francium (223) 2-8-18-32-8-1	88 Ra Radium (226) 2-8-18-32-8-2	89-103 Actinides	104 Rf Rutherfordium (261) 2-8-18-32-10-2	105 Db Dubnium (268) 2-8-18-32-10-2	106 Sg Seaborgium (266) 2-8-18-32-10-2	107 Bh Bohrium (270) 2-8-18-32-10-2	108 Hs Hassium (277) 2-8-18-32-10-2	109 Mt Meitnerium (276) 2-8-18-32-10-2	110 Ds Darmstadtium (281) 2-8-18-32-10-1	111 Rg Roentgenium (282) 2-8-18-32-10-2	112 Cn Copernicium (285) 2-8-18-32-10-2	113 Nh Nihonium (284) 2-8-18-32-10-3	114 Fl Flerovium (289) 2-8-18-32-10-4	115 Mc Moscovium (290) 2-8-18-32-10-5	116 Lv Livermorium (293) 2-8-18-32-10-6	117 Ts Tennessine (294) 2-8-18-32-10-7	118 Og Oganesson (294) 2-8-18-32-10-8

57 La Lanthanum 138.91 2-8-18-32	58 Ce Cerium 140.12 2-8-18-32	59 Pr Praseodymium 140.91 2-8-18-32	60 Nd Neodymium 144.24 2-8-18-32	61 Pm Promethium (145) 2-8-18-32	62 Sm Samarium 150.36 2-8-18-32	63 Eu Europium 151.96 2-8-18-32	64 Gd Gadolinium 157.25 2-8-18-32	65 Tb Terbium 158.93 2-8-18-32	66 Dy Dysprosium 162.50 2-8-18-32	67 Ho Holmium 164.93 2-8-18-32	68 Er Erbium 167.26 2-8-18-32	69 Tm Thulium 168.93 2-8-18-32	70 Yb Ytterbium 173.05 2-8-18-32	71 Lu Lutetium 174.97 2-8-18-32
89 Ac Actinium (227) 2-8-18-32-10-2	90 Th Thorium 232.04 2-8-18-32-10-2	91 Pa Protactinium 231.04 2-8-18-32-10-1	92 U Uranium 238.03 2-8-18-32-10-2	93 Np Neptunium (237) 2-8-18-32-10-2	94 Pu Plutonium (244) 2-8-18-32-10-2	95 Am Americium (243) 2-8-18-32-10-2	96 Cm Curium (247) 2-8-18-32-10-2	97 Bk Berkelium (247) 2-8-18-32-10-2	98 Cf Californium (251) 2-8-18-32-10-2	99 Es Einsteinium (252) 2-8-18-32-10-2	100 Fm Fermium (257) 2-8-18-32-10-2	101 Md Mendelevium (258) 2-8-18-32-10-2	102 No Nobelium (259) 2-8-18-32-10-2	103 Lr Lawrencium (260) 2-8-18-32-10-3

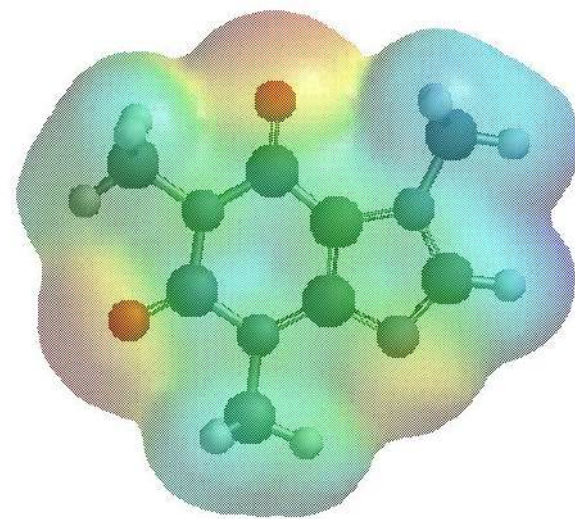
Atomic Number → 1
 Symbol → **H**
 Name → Hydrogen
 Atomic Weight → 1.008
 Electrons per shell → 1

State of matter (color of name)
 GAS LIQUID SOLID UNKNOWN

Subcategory in the metal-metalloid-nonmetal trend (color of background)
 Alkali metals Lanthanides Metalloids
 Alkaline earth metals Actinides Reactive nonmetals
 Transition metals Post-transition metals Noble gases
 Unknown chemical properties



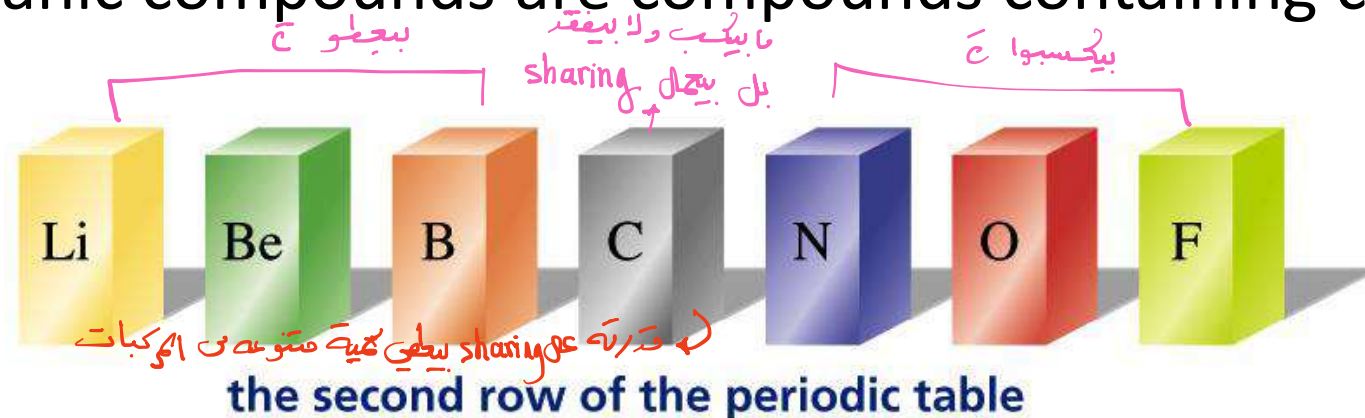
Chapter 1: Bonding and Isomerism



يعتم في المركبات التي Organic Chemistry

تحتوي على C

- Organic compounds are compounds containing carbon

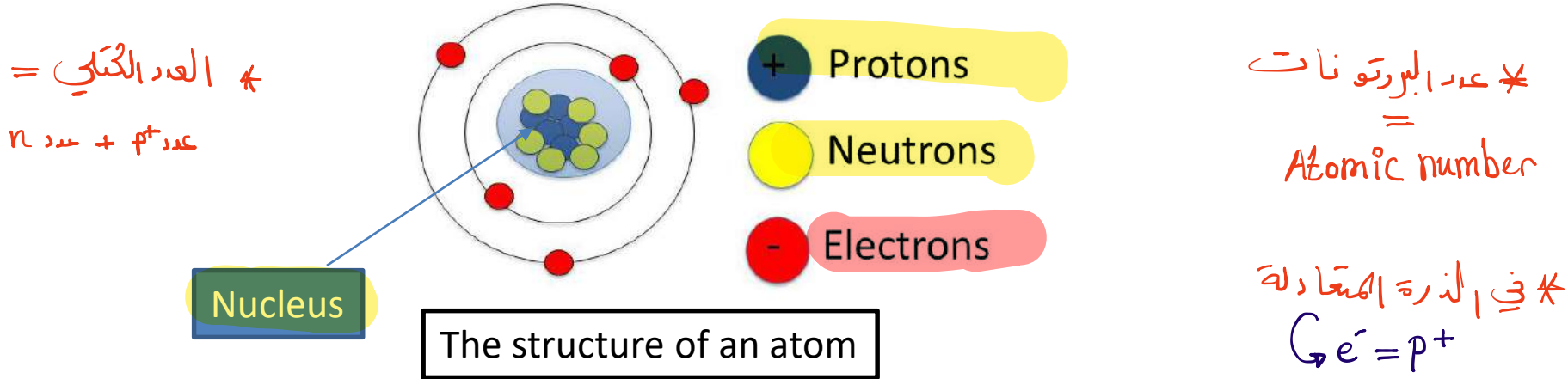


- Atoms to the left of carbon give up electrons.
- Atoms to the right of carbon accept electrons.
- Carbon shares electrons.

Bonding and Isomerism

1.1 How Electrons Are Arranged in Atoms

- An atom is: the *smallest particle* of an element that retains all of the chemical properties of that element.
- An atom consists of negatively charged electrons, positively charged protons, and neutral neutrons



- **Atomic number:** numbers of protons in its nucleus and it's the number of electrons in the neutral atom.
- **Mass number:** the sum of the protons and neutrons of an atom.
(Protons and neutrons are ~ 1837 times the mass of an e^-)
- Isotopes have the same atomic number but different mass numbers (^{12}C and ^{13}C)

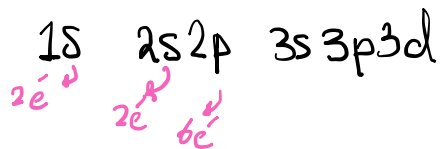
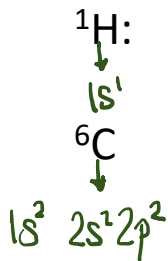
- Electrons are located in atomic orbitals (S, P, d, f).
- Orbitals tell us the energy of the electron and the volume of space around the nucleus where an electron is most likely to be found.
- Orbitals are grouped in shells .

Each orbital can hold a maximum of $2e^-$ and the two electrons have opposite spin

Table 1.1 Distribution of Electrons in the First Four Shells That Surround the Nucleus

	First shell	Second shell	Third shell	Fourth shell
Atomic orbitals	s	s, p	s, p, d	s, p, d, f
Number of atomic orbitals	1	1, 3	1, 3, 5	1, 3, 5, 7
Maximum number of electrons	2	8	18	32

Example :



* بس اجي ابعي ع
 بعني بالترتيب
 بعني اوله اتي
 وذا اكمل م

← يعني مدار
 الاول مستقرين
 اثنان من الثاني
 وهكذا

Valence electrons (VE) are located in the outermost shell. They are involved in chemical reactions.

ما موجود في آخر shell أي في آخر orbital

VE = Group number

Examples: ${}^1\text{H}: 1s^1$

VE

Lewis symbol of atom

1

H·

${}^8\text{O}: 1s^2 2s^2 2p^4$

6

·
·
O·
·
·

${}^6\text{C}: \underline{\hspace{10cm}}$

Table 1.3 Valence Electrons of the First 18 Elements

Group	I	II	III	IV	V	VI	VII	VIII
	H·							He:
	Li·	Be·	·B·	·C·	·N:	·O:	:F:	:Ne:
	Na·	Mg·	·Al·	·Si·	·P:	·S:	:Cl:	:Ar:

الترتيبة
لرسم (VE)

هو الكربون
بمجاوزه
(VE)

* الميليوم بتوي

على ١٧٤

من ٨

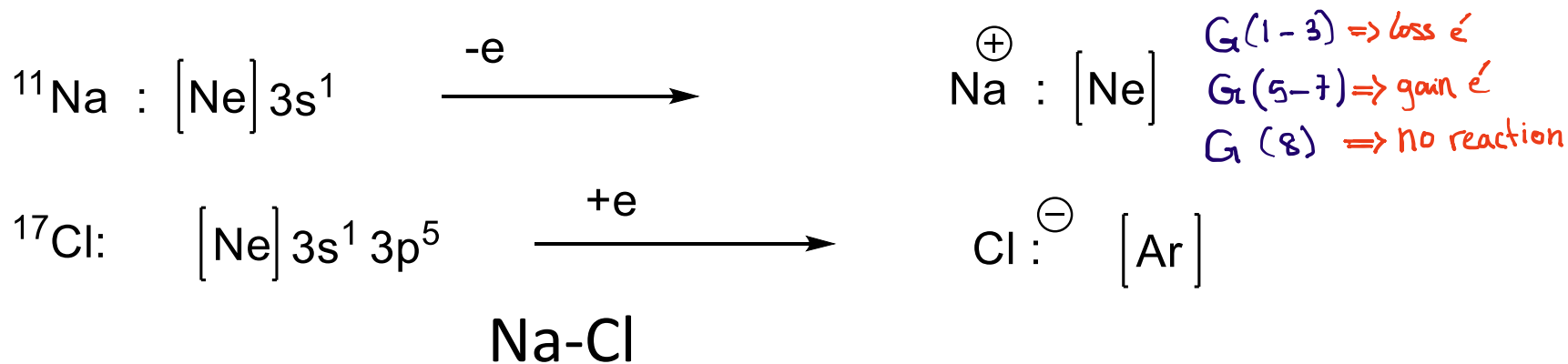
- **Chemical Bonds**

لأنه عنان كونه مع الذرة لحالة استقرار
(الحجمان مستوى التكافؤ)

1. Ionic Bonding

↳ Completely transfer of e^-

An ionic bond is an electrostatic attraction between positive & negative ions resulting from e^- transfer.



The resulting e^- configuration of both ions are those of the nearest noble gas, Ne and Ar respectively, both satisfy the octet rule.

2. Covalent Bonding

↳ sharing e⁻

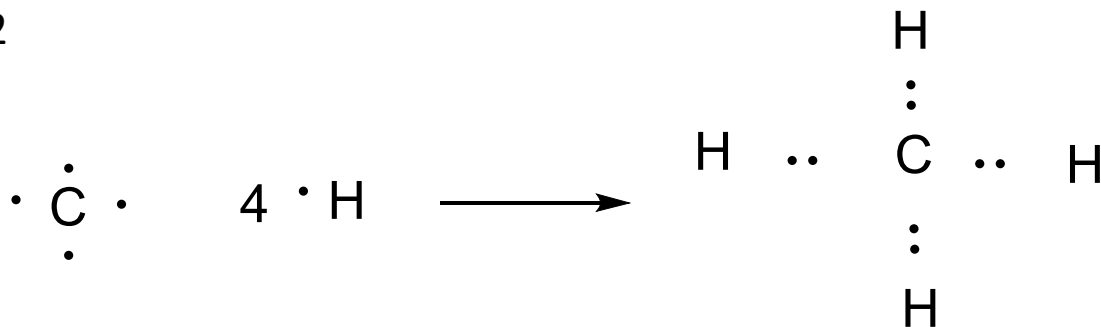
- Ionic bonds occur when an e⁻ is transferred between a metal and nonmetal.
- Covalent bonds are resulting from **sharing** e⁻



The result is both atoms have a [He] e⁻ configuration, *i.e.*

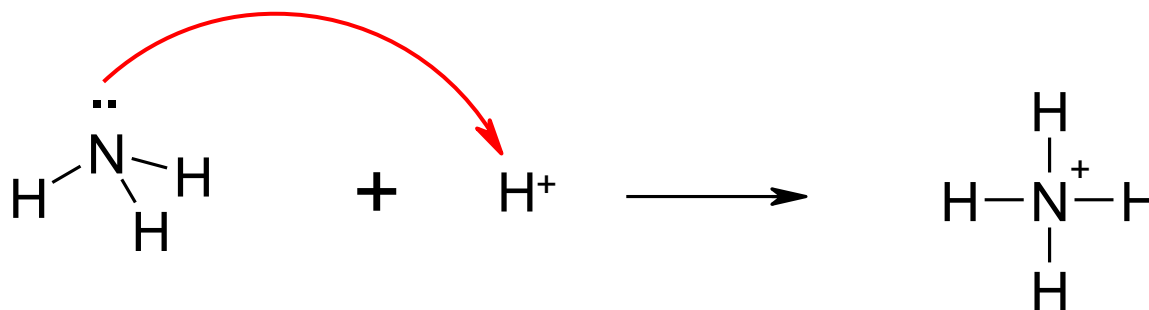
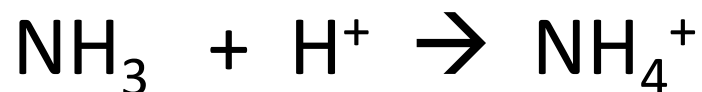
The bond is commonly display as a line rather than a pair of e⁻ (:), *i.e.* H - H rather than H : H

Example 2



A second general version of a covalent bond is possible. This occurs when BOTH e⁻ come from one atom: a **coordinate covalent bond**

i.e.



الكهروسالبية

Electronegativity (EN) : measures the tendency of an atom to attract a shared pair of electrons (or electron density).

* الذرة التي

لديها قدرة أكبر
على جذب
إلكترون

* يتم حسابها
عن طريق
الفرق بين الذرات

فكلما زاد قوة جذبها

TABLE 1.3 The Electronegativities of Selected Elements^a

IA	IIA	IB	IIB	IIIA	IVA	VA	VIA	VIIA
H 2.1								
Li 1.0	Be 1.5			B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2			Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0							Br 2.8
								I 2.5

Handwritten notes on the table:
 - A red box around H (2.1) with an arrow pointing to the difference between H and Li (-0.9).
 - Red arcs above the B, C, N, O, F row with values -0.5, -0.5, -0.5, and an arrow pointing to the difference between O and F (-0.5).
 - A red arrow at the bottom pointing right with the text "increasing electronegativity".
 - A red arrow on the right pointing up with the text "increasing electronegativity".

^aElectronegativity values are relative, not absolute. As a result, there are several scales of electronegativities. The electronegativities listed here are from the scale devised by Linus Pauling.

كل ما كان
الذرة أكبر
يزداد
إلى النواة
فكلما
على جذبها

Covalent bonds can be classified as

A. Nonpolar covalent bond ($\Delta EN = 0-0.5$)

Examples C-C C-H

Covalent bond
ما بتسام عى
ترتيب كامل
بتسام عى
bond.

polar $\Rightarrow \Delta EN = [0.5 - 1.9]$

② بخون نيه
 $+S, -S$

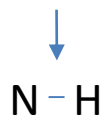
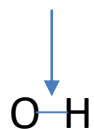
والذرة الاكثر EN هي -S

③ كل ما زاد ΔEN
تزداد القطبية

dipole moment (D) = $\mu = e \times d$

non-polar $\Rightarrow \Delta EN = [0 - 0.5]$

B. Polar covalent bond ($\Delta \text{EN} = 0.5 \text{ } 1.9$)



A polar bond has a negative end and a positive end

$$\text{dipole moment (D)} = \mu = e \times d$$

(e) : magnitude of the charge on the atom

(d) : distance between the two charges

Table 1.4 The Dipole Moments of Some Commonly Encountered Bonds

Bond	Dipole moment (D)	Bond	Dipole moment (D)
H—C	0.4	C—C	0
H—N	1.3	C—N	0.2
H—O	1.5	C—O	0.7
H—F	1.7	C—F	1.6
H—Cl	1.1	C—Cl	1.5
H—Br	0.8	C—Br	1.4
H—I	0.4	C—I	1.2

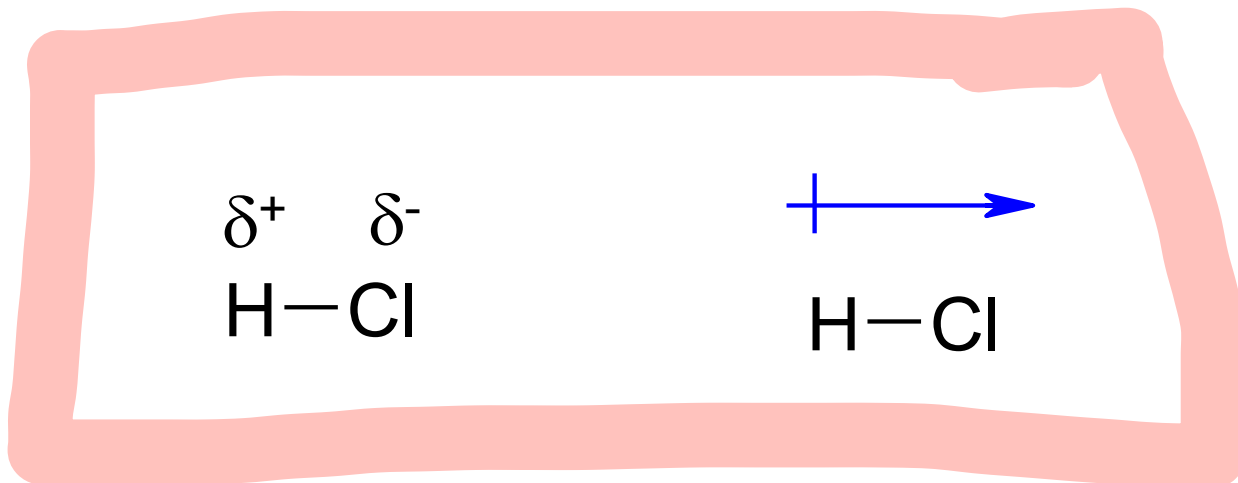
if The ΔEN increases the polarity increases

Note : If ΔEN is more than 1.9 then the bond is ionic Ex: Li-F

(1 bond)

Bond Polarity & Electronegativity (cont'd)

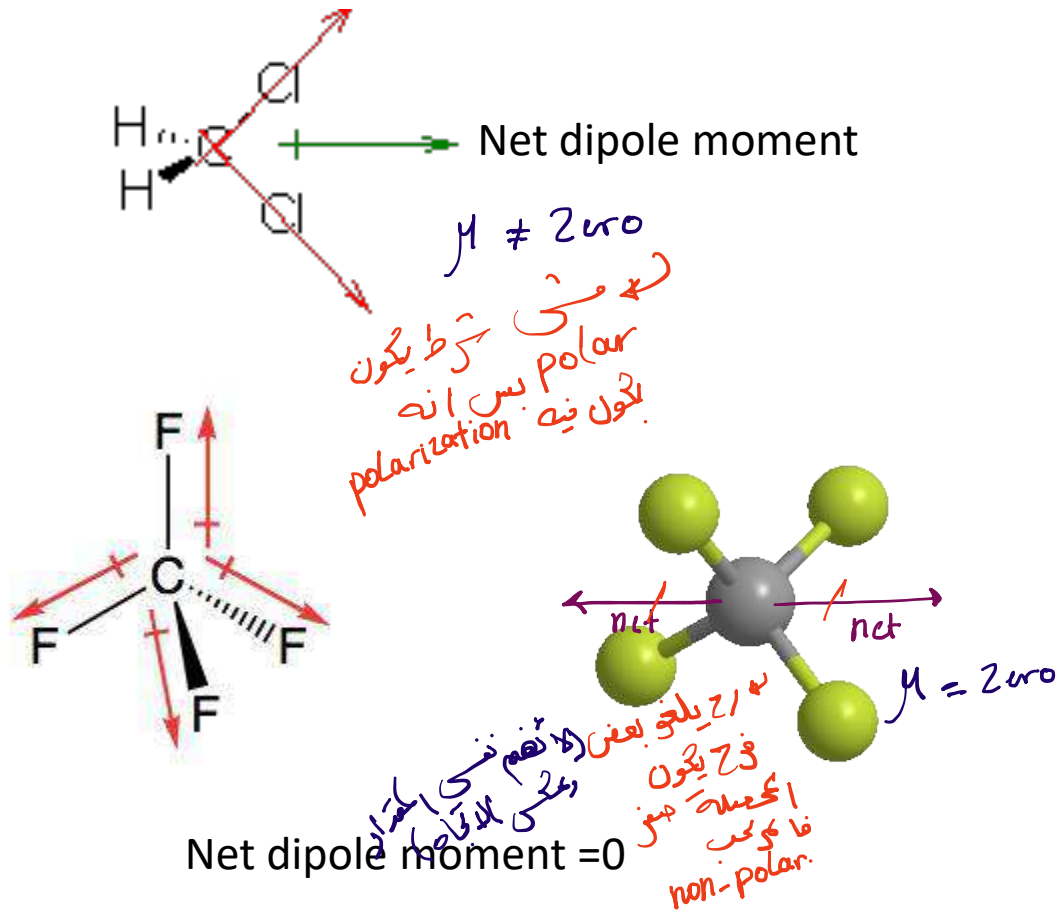
The result of polar covalent bonding is that the e^- pair spend more time near the more EN atom. This means it will acquire a permanent excess negative charge. The other atom acquires a permanent excess positive charge. This is indicated by a δ^+ or δ^- (where δ means a “partial charge”) or a dipole arrow which points from the positive end of the bond to the negative end.



(more than 1 bond)

Bond Polarity & Electronegativity (cont'd)

The more polar the molecule the stronger the dipole moment. The molecular dipole moment is the vector sum of the bond moments, *i.e.*



Lewis Structures

It only deals with VE

Procedure for obtaining good Lewis structures: eg. CO₂

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

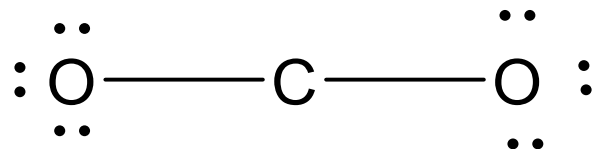
$$\text{CO}_2 = 4 + 2(6) = 16.$$

- 2) Chose a central 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.

$$16 - 4 = 12$$



VE: \bar{e} الموجود في المدار الأخير: \bar{e} [last shell] involved in chemical reaction
 [١٣٣ اي خلوا Atom يعملون lose / gain / share]

Rules 8-

① $CO_2 = C(4) + O_2(2 \times 6) = 16 e^-$ → احدد التوتال نمبر لل VE الي موجودين بالمركب

② $\Rightarrow C$ هون
 اختار ال central atom وهي الي بتكون عندها اقل كهروسالبية (الي بتقدر تعمل اكثر عدد روابط)

③ $O \quad C \quad O$
 بوزع other atoms حول central atom

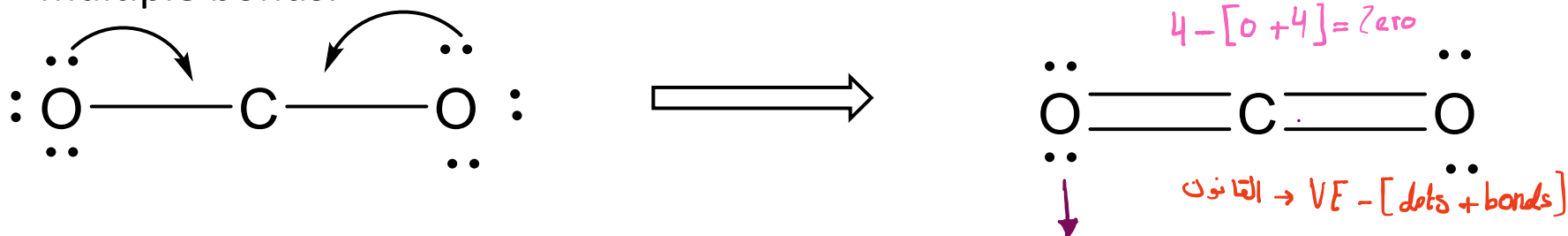
④ $O - C - O$
 يعمل single bond بين central atom و other atom
 لو مسه بكون اخذت 4e
 في اعمل 16e

⑤ $:\ddot{O} - C - \ddot{O}:$
 بوزع باقي الالكترونات على الذرات الباقية

⑥ هون عندي C هي الي عشان الذرة تكون في حالة استقرار لازم يكون عندها 8 الكترونات في المدار الاخير (في استثناءات بس مش داخله معنا) فبشيك عكل ذرة انه صار عندها 8 →

⑦ بجيب الكترونات زيادة عن طريق اني اسحب زوج الكترونات من الذرات الثانية و اشاركهم مع الذرة الي عنها نقص فبتكون رابطة $:\ddot{O} = C = \ddot{O}:$

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



5) determine the formal charges of all atoms. له بحسب رقم

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

بعد ما رسمت لويس structure حتى اتأكد انه رسمي
 صح رح اشوف formal charges والي هي ال

المركب ال neutral بتكون الشحنة الكلية تبعته

For O $6 - 6 = 0$

For C $4 - 4 = 0$

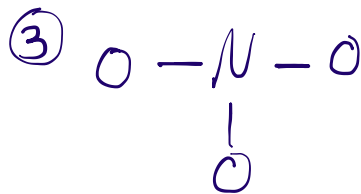
VE $\rightarrow 6e^-$
 Group $6 - [4 + 2] = Zero$

بِسبَبِ اِىِ عَالِ الْمُرَكَّبِ [اِكْتَسَبَ عَ]

Ex: NO_3^-

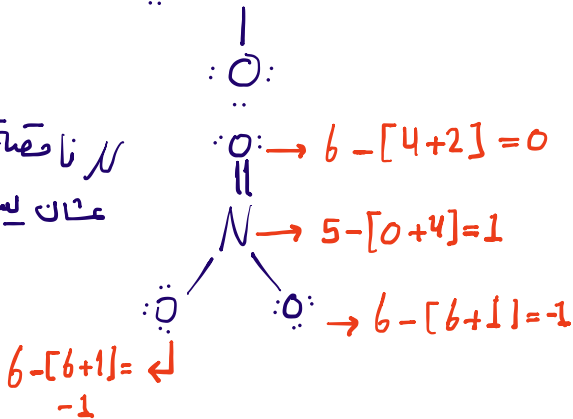
① $VE = 5 + [6 \times 3] + \underline{1} = 24$

② Central Atome $\rightarrow \text{N}$



④ باقى 18 ع $\text{:}\ddot{\text{O}} - \text{N} - \ddot{\text{O}}\text{:}$

⑤ ن ناقصه 2 ع
عنان لستقر



Total charges = $1 - 1 - 1 = -1$

هذا هو الجواب

1. $VE = 5 + 6 \times 3 + 1 = 24$

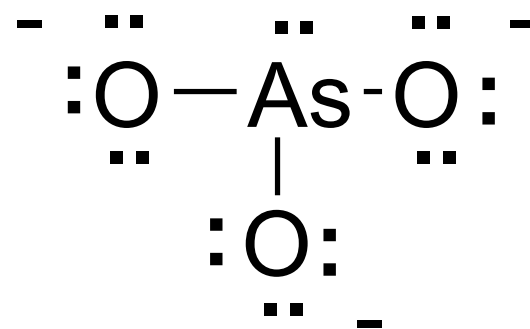
$5 + 6(3) + 1$

24

Lewis Structures (other examples)

Example 2: AsO_3^{3-}

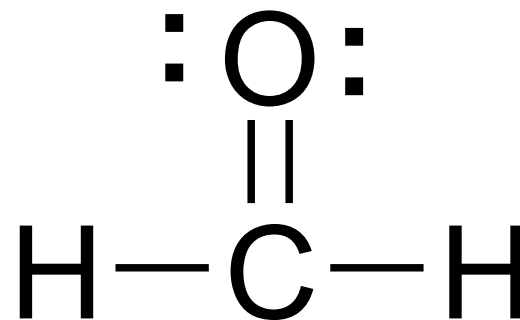
- 1) # e^- : $5 + 3(6) + 3 = 26$
- 2) form 3 single bonds
- 3) 20 e^- remain
- 4) O needs 6, As needs 2
- 5) All octets
- 6) Formal charges



Lewis Structures (cont'd)

Example 3: CH₂O

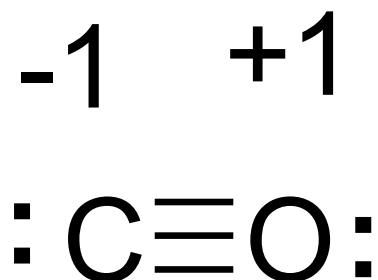
- 1) # e⁻: 4 + 2(1) + 6 = 12
- 2) try 3 single bonds
- 3) 6 e⁻ remain
- 4) O 6 but C?
- 5) Form a double bond
- 6) Both O & C octets
- 7) Formal charges



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

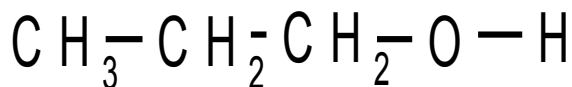


1.8 Isomers

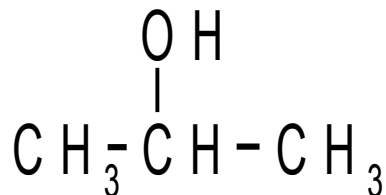
فيه اختلاف بالخصائص الفيزيائية والكيميائية. مركبات الهم نفس ال molecular formula لكن يختلفو
عن بعض في structural formula بينهن

Structural or constitutional isomers have same molecular formula but different structural formula. لم لنفس المصطلح

They have different physical and chemical properties:



1-propanol
(bp 97.4 C)



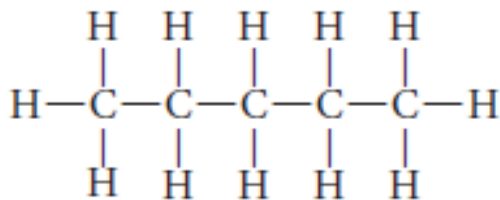
2-propanol
(bp 82.4 C)

1.9 Writing Structural Formulas

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



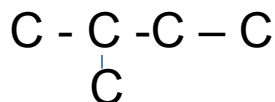
Continuous chain



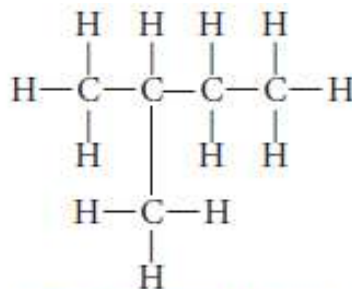
pentane, bp $36^\circ C$

Continuous chain

C forms 4 covalent bonds



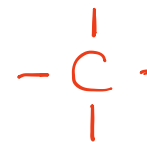
Branched chain



2-methylbutane, bp $28^\circ C$
(isopentane)

branching.

في العادة C يتصل 4 روابط بين تكون
Neutral chain



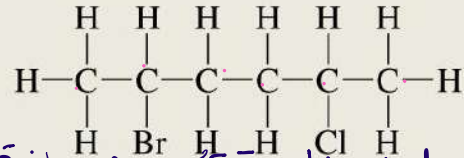
اذا بدى اعمل Isomers من نفس المركب
ممکن انه يمون contineus يعني مستمر
او ممکن يكون في branching يعني تفرع
هدول بكونو structural Isomers

في عندي اكثر من لكتابة ورسم

Dash formula

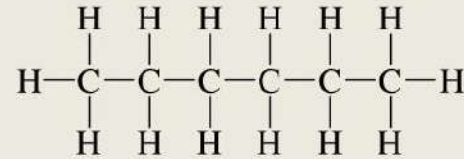
Kekul structure

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

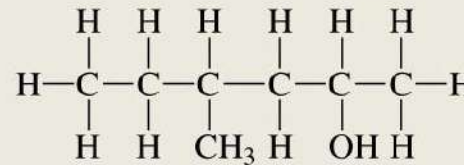


لما يكون عندي branching هاي الطريقة تكون مشي ناعمة

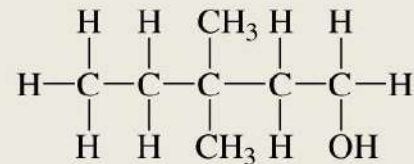
Repeating CH₂ groups can be shown in parentheses.



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

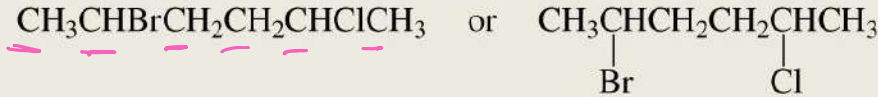


Groups bonded to the far-right carbon are not put in parentheses.



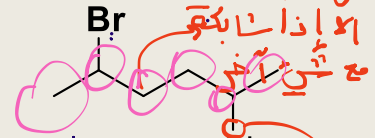
Condensed structures

Condensed structure → bond يعني



Bond line formula

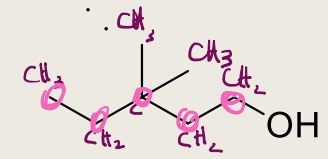
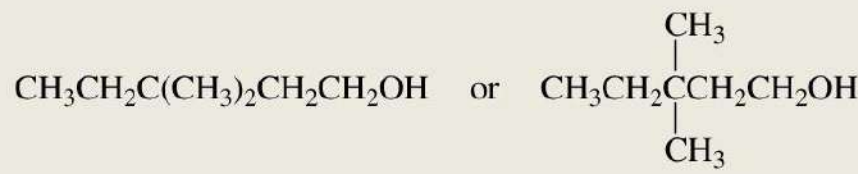
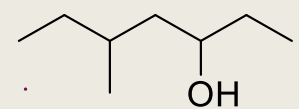
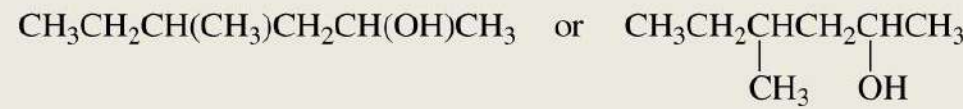
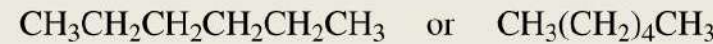
Bond line formula

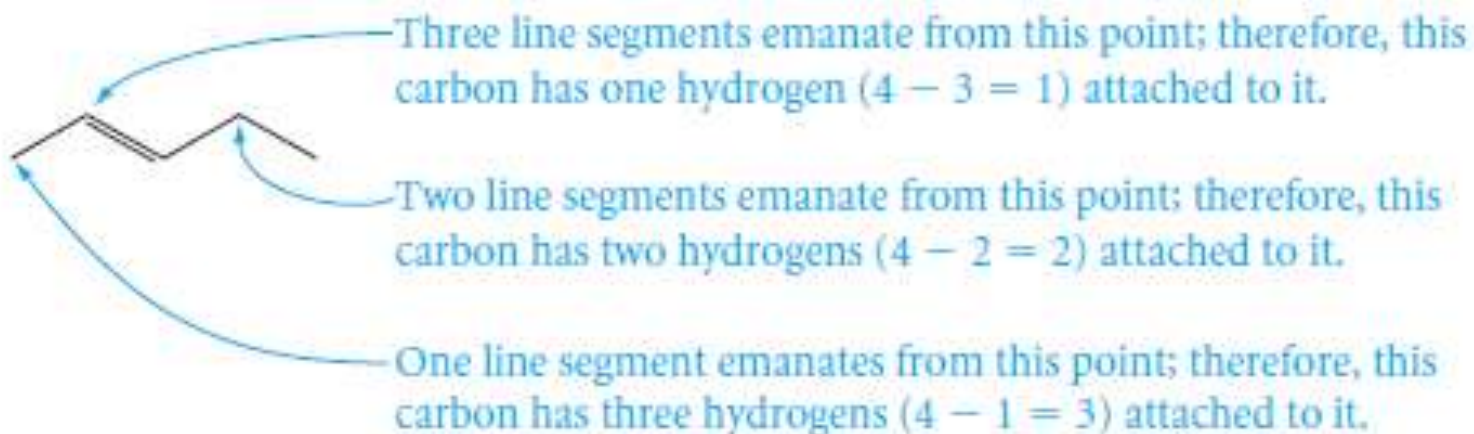


كل نقطة اوا اذا شا بقو مع شي اخر
 لا ما نطلع
 ملامهون
 هاي مشي
 ولا نطلع اليمين

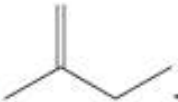
فقط نطلع bonds

- عشان اعرف عدد H
 بطلع 4 من عدد
 رابطاتي عا طليتها C

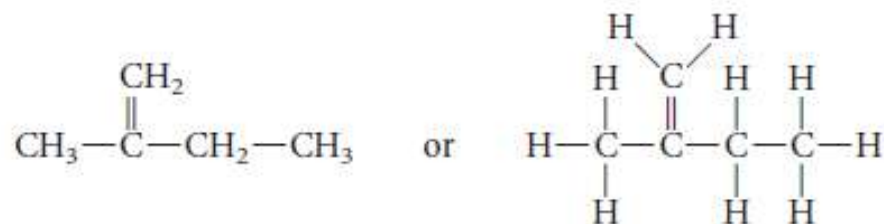




EXAMPLE 1.12

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

Covallant bond: sharing of e^-

يكونوا مطولين في orbitals [متممين في s, p]

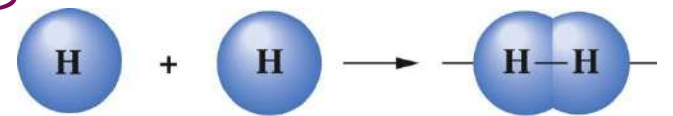
Sigma (σ) bonds: are

characterized by a region of high e^- density along the internuclear axis.

head to head يعني سيجمما (σ)

ممكن يكون بين $sp / 2p / 2s$ لكن اجمع يكون فيه منطقة تداخل حقيقي بين هذين orbitals

يكون الرابطة عن طريق ابي اعمل تداخل في orbitals



1s atomic orbitals

s-s molecular orbital



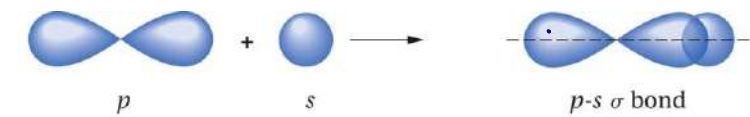
1s atomic orbital

molecular orbital

لعمل تداخل بين p, p, و لكن صدر orbital لازم انهم يكونوا [Side to side]

parallel to each other

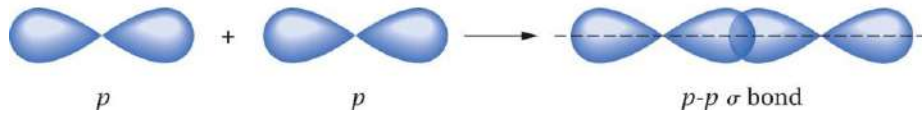
يعني اذا كان واحد في px لازم الثاني برجهه يكون في px ما يكون تداخل مباشر



p

s

p-s sigma bond



p

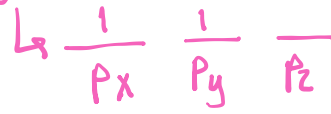
p

p-p sigma bond

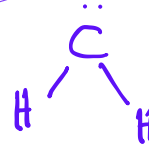
Orbitals approach each other in a **head to head** fashion

أقل طاقة من 2p
 توزيع C → 1s², 2s² 2p²

كـ بـ لـ سـ تـ باء 1s
 بالأردل هناك
 energy level
 تابعه أقل

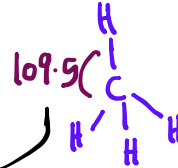
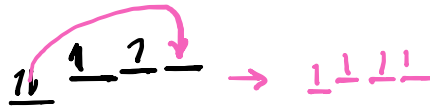


يعني مثلا بقدر
 امكن انه



شي الشكل

الموجود لـ C بل مثلا
 للمثيل اي هو أبسط
 مركب يكون

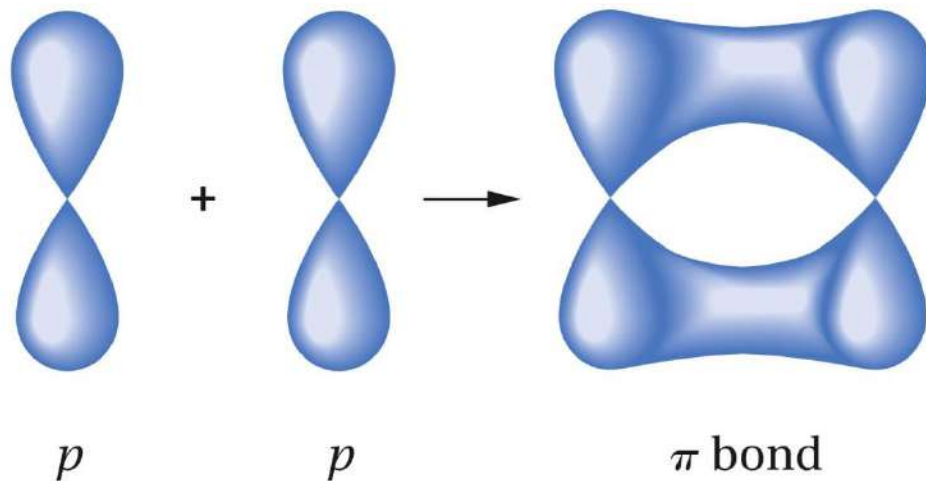


السبب انه واحد من e انطلق عند Pz وصارما يسمى free promotion بس ما وفقت لهون لانه لو لو وفقت لهون كان لقينا انه في واحد فيهم مختلفتم ربط النظرية الي هي hybridization انه انا بعمل عملية mixing لل S مع 3 p بخلط orbital s مع p_x p_y p_z ويطلع orbitals متساويين في الطاقة ومتساويين في الشكل وكل واحد فيهم اسمه Sp³ لانه انا عملت mixing لل S مع ثلاثة P

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

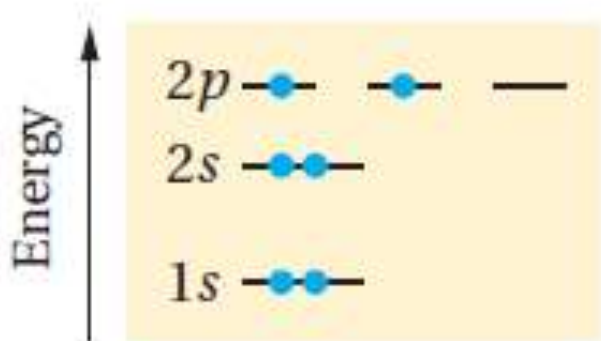
There is one other type of bond, a **pi (π) bond**. In contrast to a sigma bond the e^- density in a pi bond is not located on the internuclear axis, but rather on either “side” of it.

π bonds are formed by the side to side overlap of 2 “p” orbitals



Carbon sp^3 Hybrid Orbitals

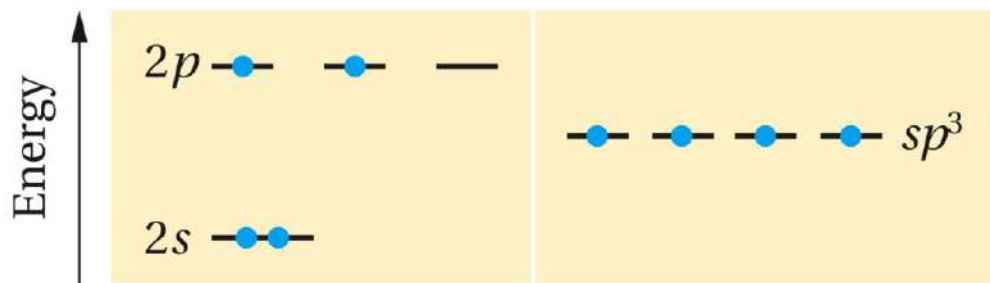
${}^6\text{C}: 1s^2 2s^2 2p^2$



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

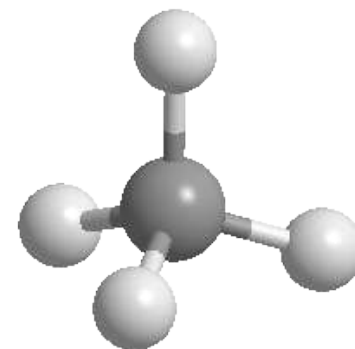
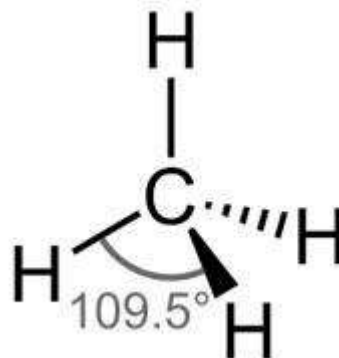
Q: Should the carbon form only two bonds !!!

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



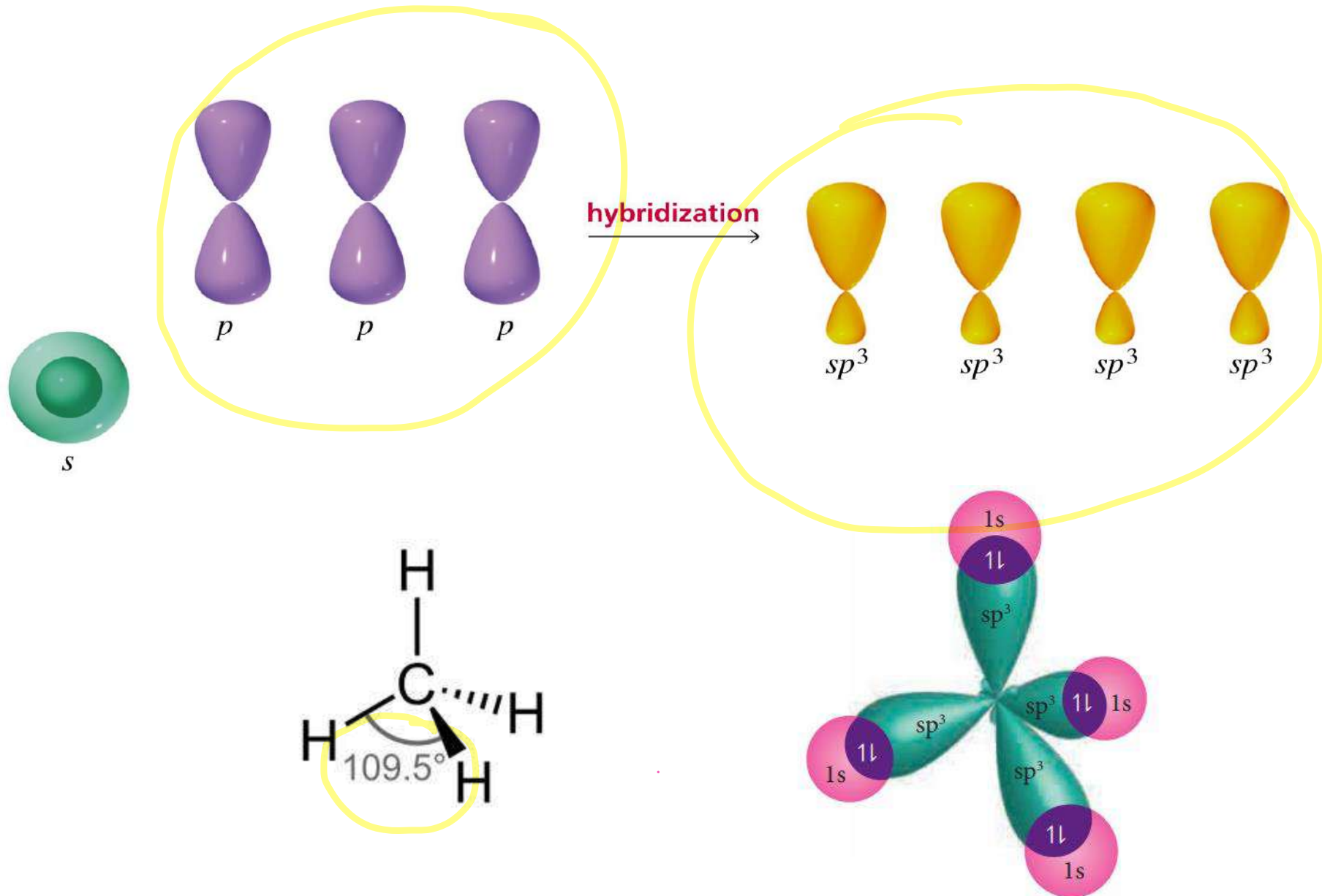
Atomic orbitals of carbon

Four equivalent sp^3 hybrid orbitals



3D Structure of Methane Molecule

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

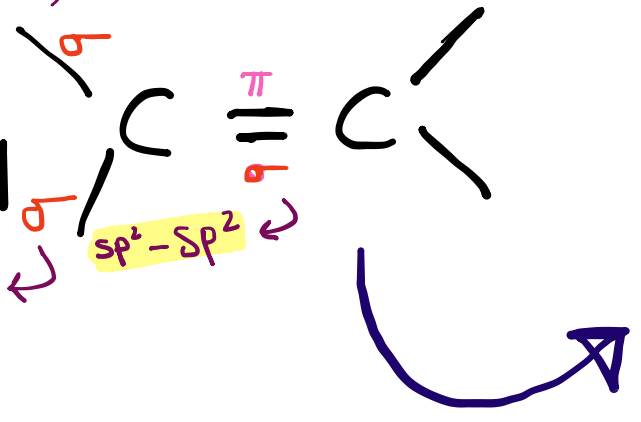


هون / آتكون

$s + sp^2$

الايثين

$s + sp^2$



$$\begin{matrix} \frac{1}{s} & \frac{1}{p_x} & \frac{1}{p_y} & \frac{1}{p_z} \end{matrix}$$

hybridization

$[sp^2]$

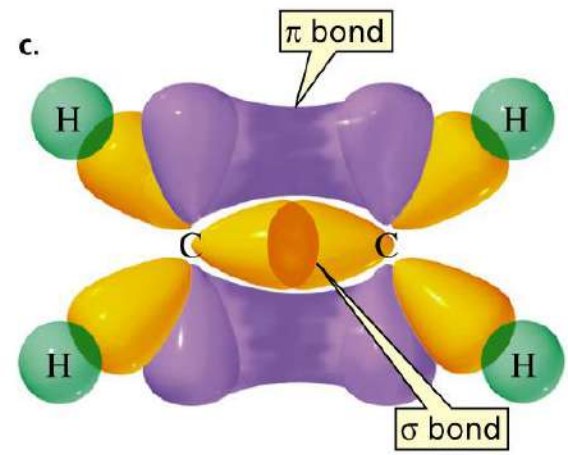
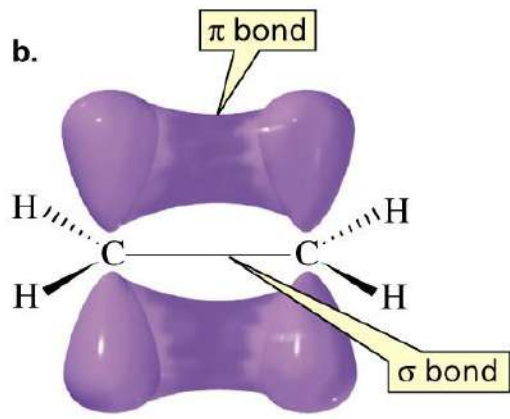
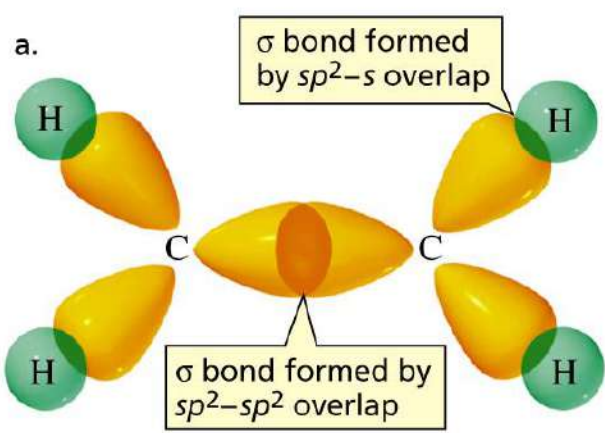
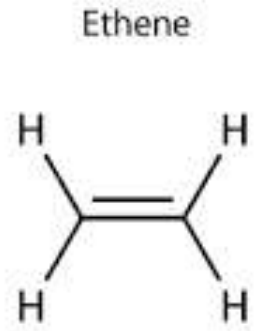
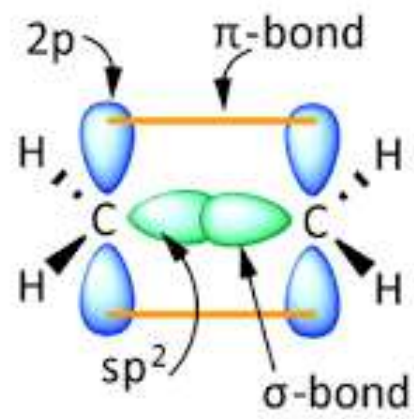
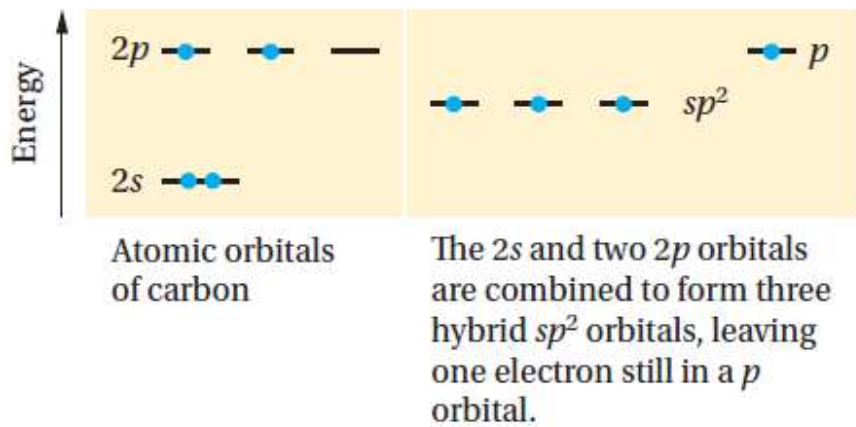
$\hookrightarrow 3\sigma$

For π

p, p orbitals parallel $\hookrightarrow \pi$
من C_1, C_2

SP²-Hybridized orbitals

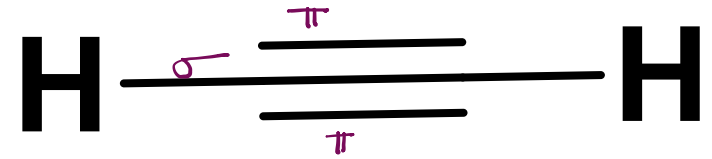
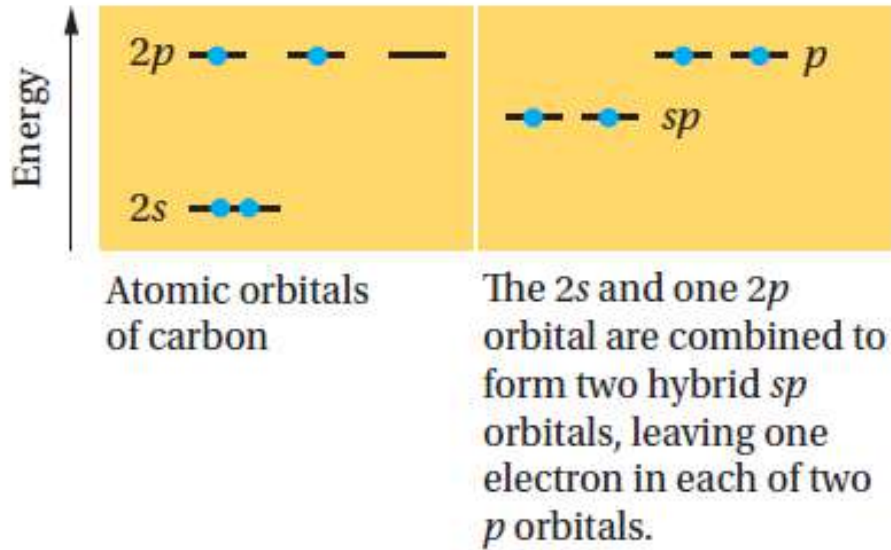
One part *s* and two parts *p* in character and are directed toward the three vertices of an equilateral triangle.



SP-Hybridized orbitals

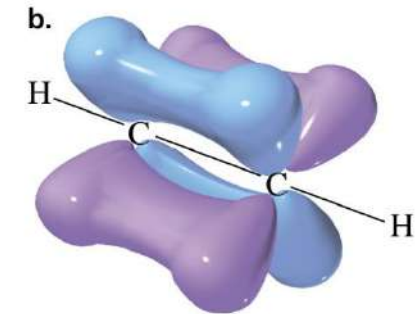
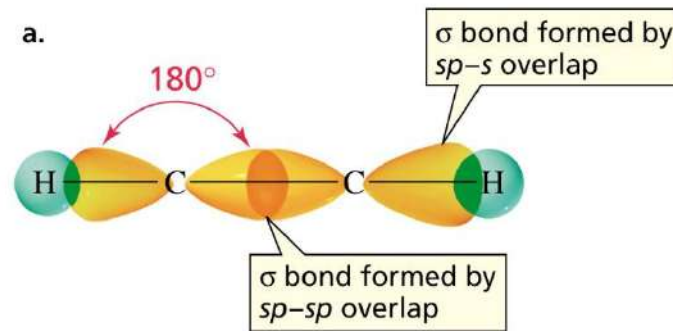
Bonding in Ethyne: A Triple Bond

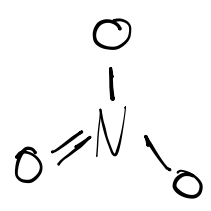
- A triple bond consists of one σ bond and two π bonds



$\pi \rightarrow$ one orbital
[σ, π, π]
 $2\pi \rightarrow 2p$ orbital

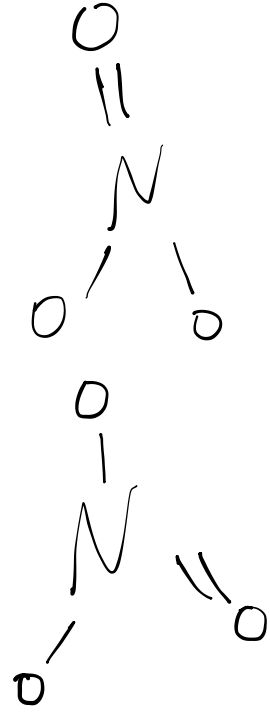
sp orbitals forms a sigma bond between the two carbons, and lateral overlap of the properly aligned p orbitals forms two pi bonds





هدول الرسومات كلهم صح بس اهم اشئ انه الرابطة الثنائىة تكون اقصر

فعليا عملية الاختلاف هون او عنلية انى ارسم diffrent لوييس ستركتشر بكون



الى بغير مكان الرابطة الثنائىة هو تغير مكان الالكترونات

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

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.

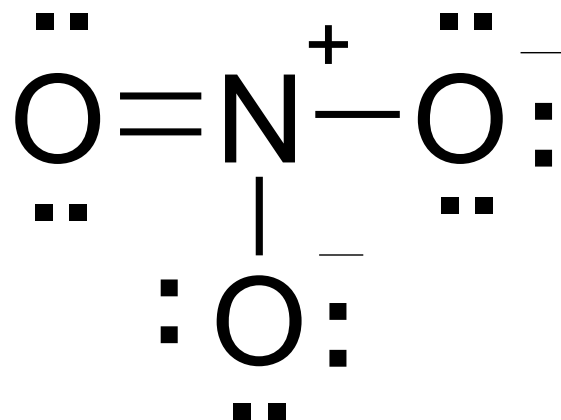
The assumption in these diagrams is that the atom positions do not change, we are only allowed to change the distribution of e^- , *i.e.* the bonds and lone pairs.

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 charges



Resonance: double bond. اختلاف مواقع

بقدر احكي انه انا في عندي resonance structure لما يكون عندي اختلاف في position of e وانا عندي نوعين من الالكترونات الي بختلف مكانهم :

هدول الالكترونات بدهم >---- (e) like double /triple bond . long pair 1:

sp²/sp يروحو على ذرة شرط يكون تهجينها

الsp³ ما بتزبط لانه رح يكون حوالين C فيه 5e

قال 2 :

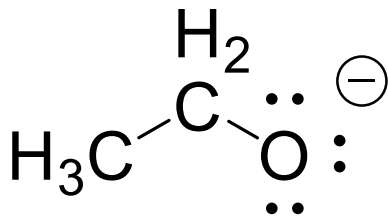
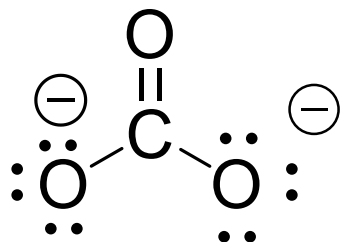


The Lewis structure can be converted to other by changing the position of electrons

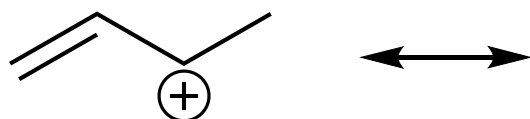
Rules for drawing resonance structures :

- 1) Electrons only can be moved (lone pair / π electrons)
- 2) Electrons move toward SP/ SP² hybridized atom only.

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



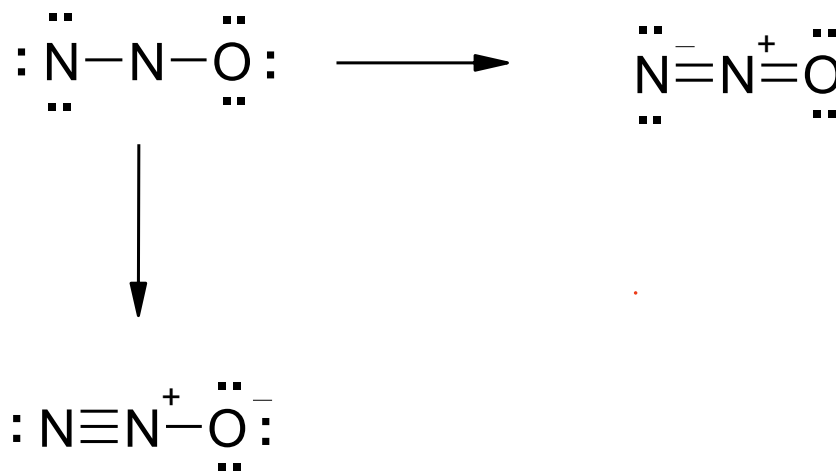
Exercise



Resonance (cont'd)

Example 2: N₂O

- 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

حسب نوعنا وشغلتيين :

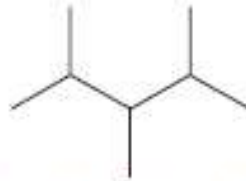
- The three main classes of molecular frameworks for organic structures are **acyclic**, **carbocyclic**, and **heterocyclic** compounds.

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

لے بد دن چلتا ہے



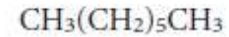
unbranched chain of eight carbon atoms



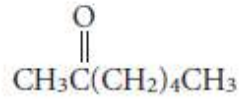
branched chain of eight carbon atoms



geraniol
(oil of roses)
bp 229–230°C



heptane
(petroleum)
bp 98.4°C



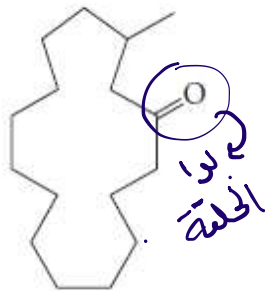
2-heptanone
(oil of cloves)
bp 151.5°C

1.17b: Carbocyclic Compounds: contain rings of carbon atoms

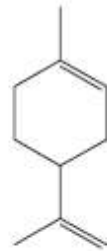
لے چلکتا اچھون
الآسی الفا
C.H

1

ما بعضی الی برا
الحلقة



muscone
(musk deer)
bp 327–330°C

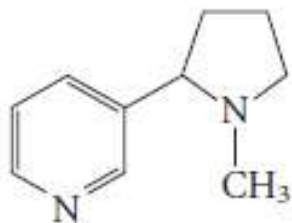


limonene
(citrus fruit oils)
bp 178°C

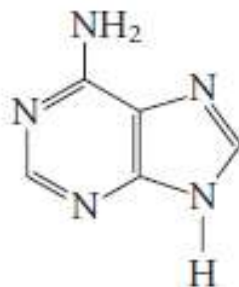


benzene
(petroleum)
mp 5.5°C, bp 80.1°C

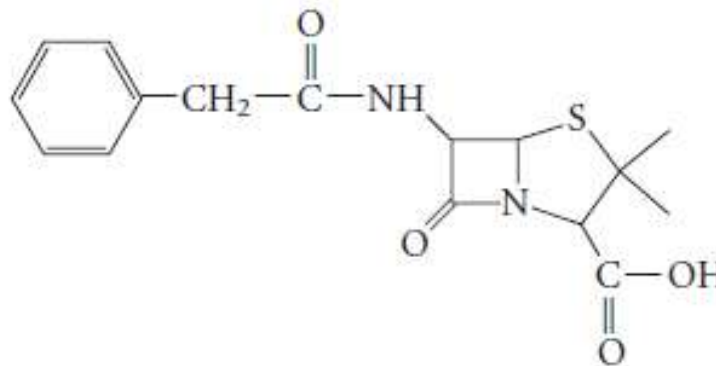
1.17.c Heterocyclic Compounds (In heterocyclic compounds, at least one atom in the ring must be a heteroatom, an atom that is *not* carbon: eg. N, O,S...)



nicotine
bp 246°C



adenine
mp 360–365°C
(decomposes)



penicillin-G
(amorphous solid)

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


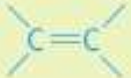



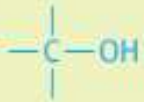
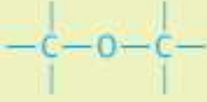
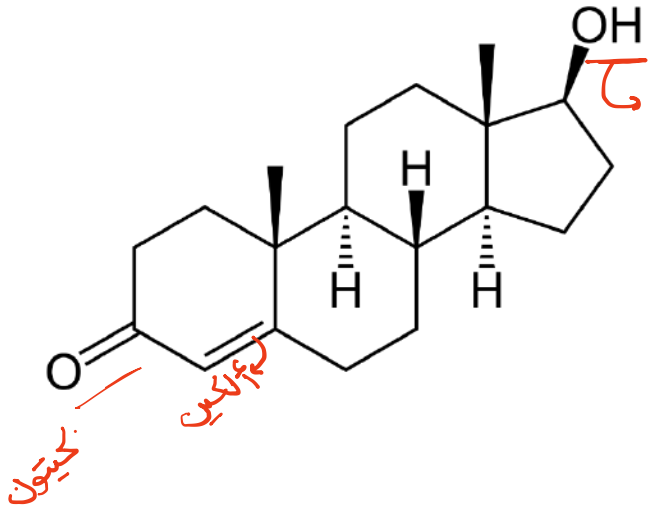
Atom موجودین مرتبہم حسب Structure	Class of compound	Specific example	Common name of the specific example
A. Functional groups that are a part of the molecular framework			
	alkane	CH ₃ —CH ₃	ethane, a component of natural gas
	alkene	CH ₂ =CH ₂	ethylene, used to make polyethylene
	alkyne	HC≡CH	acetylene, used in welding
	arene		benzene, raw material for polystyrene and phenol
B. Functional groups containing oxygen			
1. With carbon–oxygen single bonds			
	alcohol	CH ₃ CH ₂ OH	ethyl alcohol, found in beer, wines, and liquors
	ether	CH ₃ CH ₂ OCH ₂ CH 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 ₃ C(=O)CH ₃	acetone, a solvent for varnish and rubber cement
3. With single and double carbon–oxygen bonds		carboxylic acid	CH ₃ C(=O)OH	acetic acid, a component of vinegar
		ester	CH ₃ C(=O)OCH ₂ CH ₃	ethyl acetate, a solvent for nail polish and model airplane glue
C. Functional groups containing nitrogen**		primary amine	CH ₃ CH ₂ NH ₂	ethylamine, smells like ammonia
		nitrile	CH ₂ =CH—C≡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	—X	alkyl or aryl halide	CH ₃ Cl	methyl chloride, refrigerant and local anesthetic
F. Functional groups containing sulfur†		thiol (also called mercaptan)	CH ₃ SH	methanethiol, has the odor of rotten cabbage
		thioether (also called sulfide)	(CH ₂ =CHCH ₂) ₂ S	diallyl sulfide, has the odor of garlic

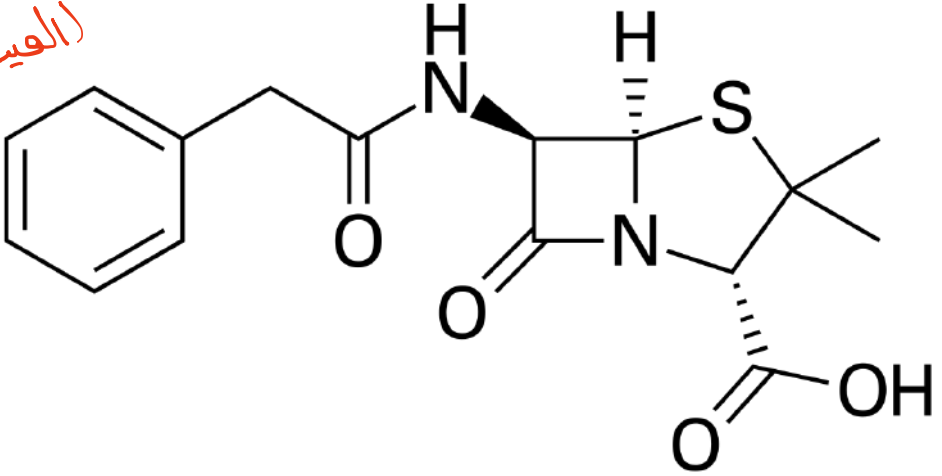


Ex. What functional groups can you find in the following natural products?



testosterone

الكحول
(الغيدروكسيل)



penicillin-G