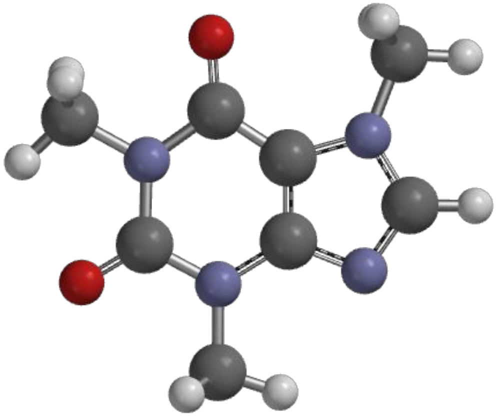
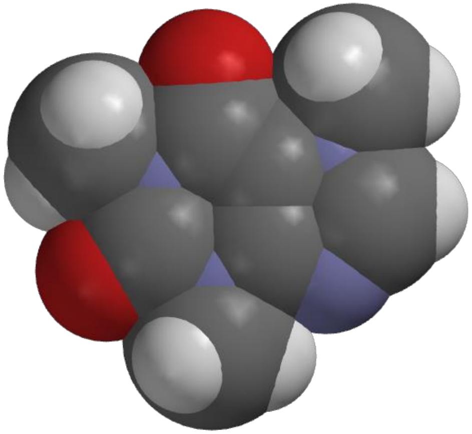
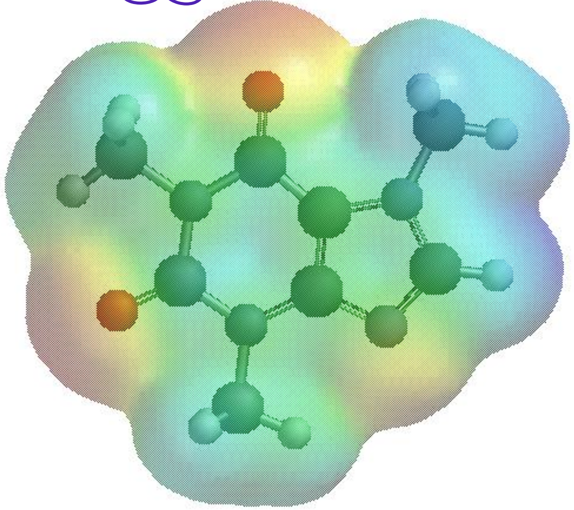




Chapter 1: Bonding and Isomerism

تفريغ

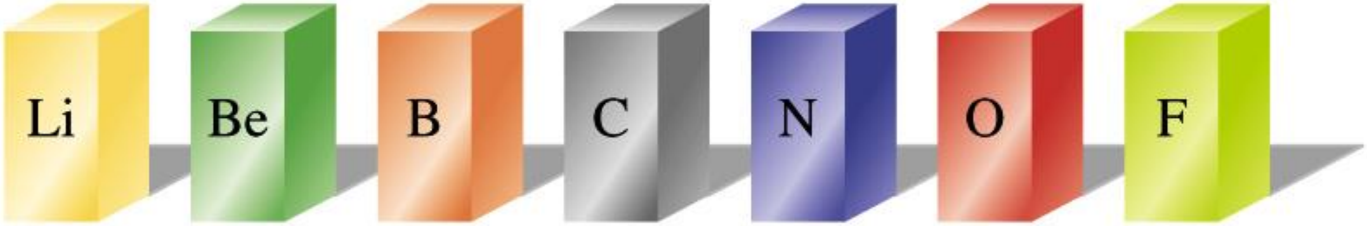
Done By : Jad Melhem



Organic Chemistry

- Organic compounds are compounds containing carbon

* carbon is a special element → it shares e^- which leads to a variety of compounds
تنوع



the second row of the periodic table

gives e^- Li^+, Be^+ B^+

recieves e^-

- 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

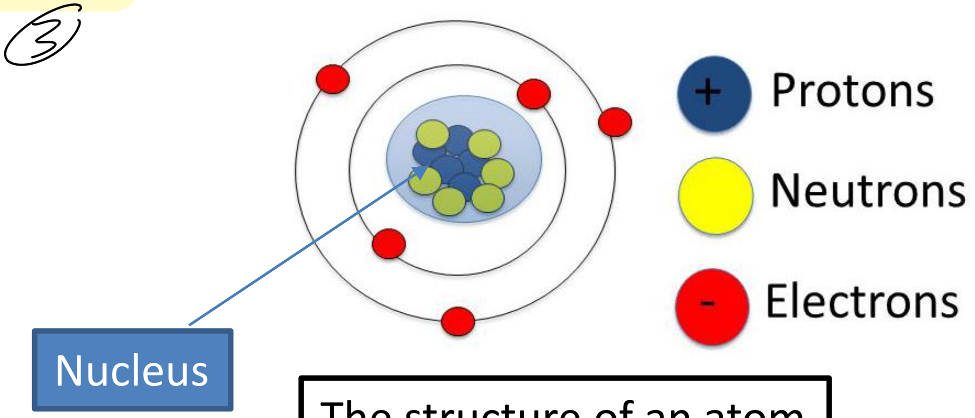
(holds)

- An atom is: the *smallest particle* of an element that retains all of the chemical properties of that element.

①　②

- An atom consists of negatively charged electrons, positively charged protons, and neutral neutrons

③



p + n

The structure of an atom

=

- **Atomic number**: numbers of protons in its nucleus and it's the number of electrons in the neutral atom.

atom كتلة ال

- **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)

نظائر　same number of (protons)　different in number of neutrons

أكبر طاقة f
اصغر طاقة s

where e⁻ are found

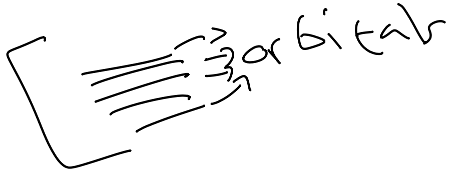
- Electrons are located in atomic orbitals (S, P, d, f).

(مدارات)

the farthest the shell is from nucleus → the higher the energy (PE)

- 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 .

shell



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

* the atomic orbital (s) can only hold 2e⁻ max. but, (p) can hold up to 6 e⁻

Example :

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

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

(توزيع e⁻)

from it we can know (V.e) group number which can also be known from periodic table (easier)

آخر shell وليس آخر orbital

Valence electrons (VE) are located in the outermost shell. They are involved in chemical reactions. ex: carbon has 4 V.e , hydrogen has 1 V.e , Oxegen has 6 V.e

VE = Group number (from ssps ps.... $\boxed{\text{or}}$ periodic table)

		VE	Lewis symbol of atom
Examples:	^{1}H: Is^{1}	1	H·
	^{8}O: $IS^{2}\ 2S^{\textcircled{2}}\ 2P^{\textcircled{4}}$	6	$\ddot{\underset{\cdot\cdot}{O}}:$
	^{6}C: ________________________________		

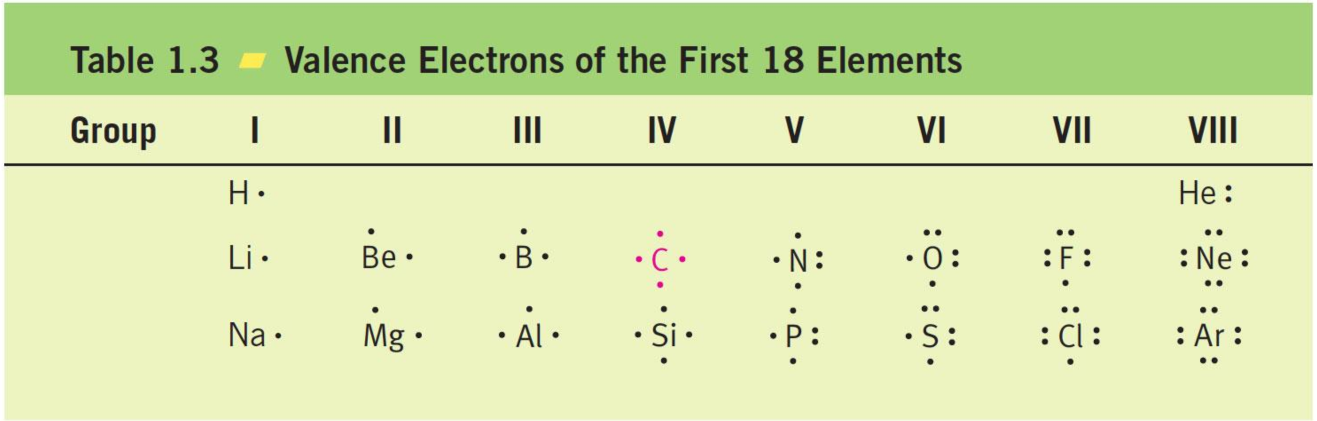
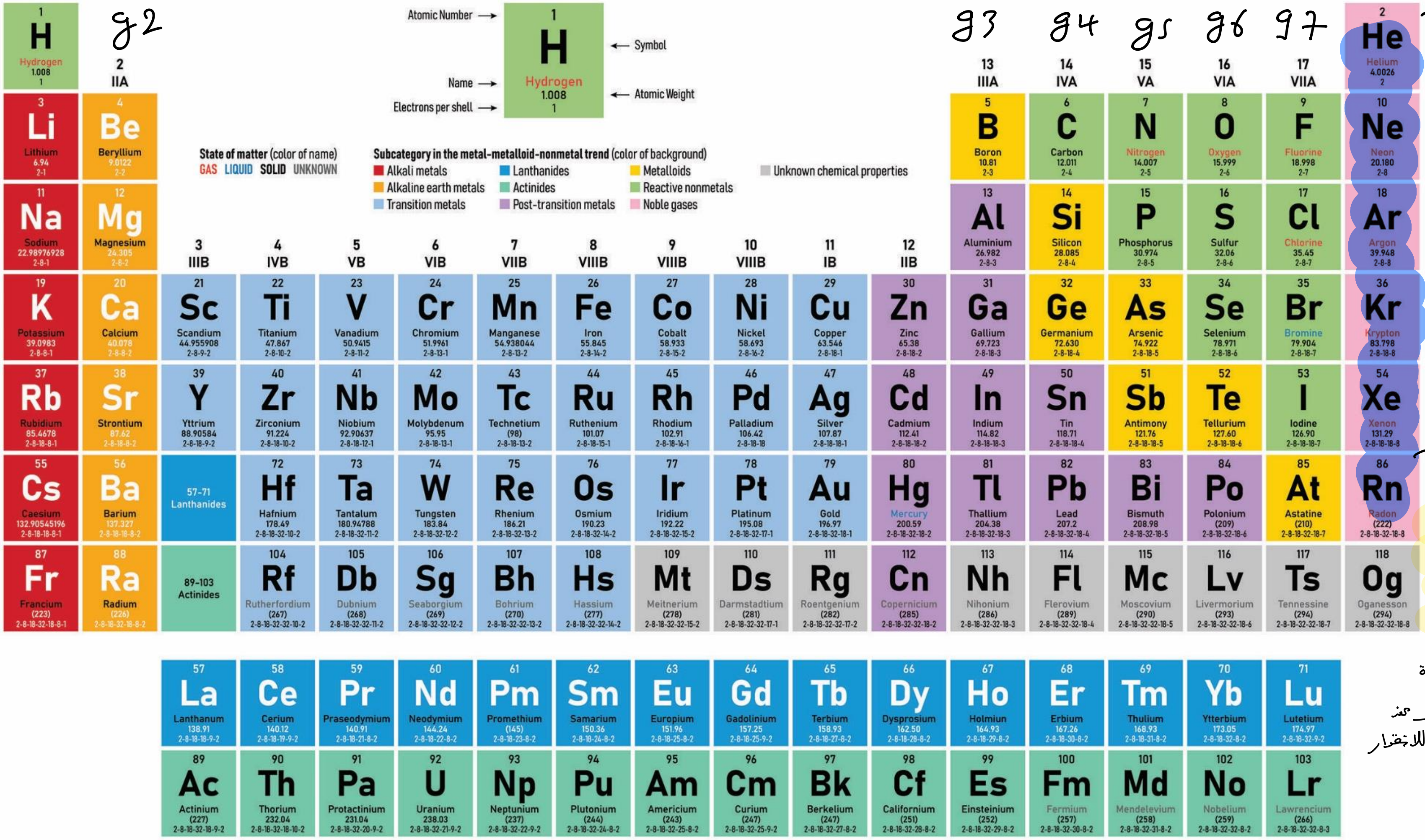


Table 1.3 ▰ **Valence Electrons of the First 18 Elements**

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 :

(dots resemble V.e)

Periodic Table of the Elements



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
- ■ Alkaline earth metals
- ■ Transition metals
- ■ Lanthanides
- ■ Actinides
- ■ Post-transition metals
- ■ Metalloids
- ■ Reactive nonmetals
- ■ Noble gases
- ■ Unknown chemical properties

g1 1 IA	g2 2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	g3 13 IIIA	g4 14 IVA	g5 15 VA	g6 16 VIA	g7 17 VIIA	g8 18 VIIIA
1 **H** Hydrogen 1.008 1																	2 **He** Helium 4.0026 2
3 **Li** Lithium 6.94 2-1	4 **Be** Beryllium 9.0122 2-2											5 **B** Boron 10.81 2-3	6 **C** Carbon 12.011 2-4	7 **N** Nitrogen 14.007 2-5	8 **O** Oxygen 15.999 2-6	9 **F** Fluorine 18.998 2-7	10 **Ne** Neon 20.180 2-8
11 **Na** Sodium 22.98976928 2-8-1	12 **Mg** Magnesium 24.305 2-8-2											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
19 **K** Potassium 39.0983 2-8-8-1	20 **Ca** Calcium 40.078 2-8-8-2	21 **Sc** Scandium 44.955908 2-8-9-2	22 **Ti** Titanium 47.867 2-8-10-2	23 **V** Vanadium 50.9415 2-8-11-2	24 **Cr** Chromium 51.9961 2-8-13-1	25 **Mn** Manganese 54.938044 2-8-13-2	26 **Fe** Iron 55.845 2-8-14-2	27 **Co** Cobalt 58.933 2-8-15-2	28 **Ni** Nickel 58.693 2-8-16-2	29 **Cu** Copper 63.546 2-8-18-1	30 **Zn** Zinc 65.38 2-8-18-2	31 **Ga** Gallium 69.723 2-8-18-3	32 **Ge** Germanium 72.630 2-8-18-4	33 **As** Arsenic 74.922 2-8-18-5	34 **Se** Selenium 78.971 2-8-18-6	35 **Br** Bromine 79.904 2-8-18-7	36 **Kr** Krypton 83.798 2-8-18-8
37 **Rb** Rubidium 85.4678 2-8-18-8-1	38 **Sr** Strontium 87.62 2-8-18-8-2	39 **Y** Yttrium 88.90584 2-8-18-9-2	40 **Zr** Zirconium 91.224 2-8-18-10-2	41 **Nb** Niobium 92.90637 2-8-18-12-1	42 **Mo** Molybdenum 95.95 2-8-18-13-1	43 **Tc** Technetium (98) 2-8-18-13-2	44 **Ru** Ruthenium 101.07 2-8-18-15-1	45 **Rh** Rhodium 102.91 2-8-18-16-1	46 **Pd** Palladium 106.42 2-8-18-18	47 **Ag** Silver 107.87 2-8-18-18-1	48 **Cd** Cadmium 112.41 2-8-18-18-2	49 **In** Indium 114.82 2-8-18-18-3	50 **Sn** Tin 118.71 2-8-18-18-4	51 **Sb** Antimony 121.76 2-8-18-18-5	52 **Te** Tellurium 127.60 2-8-18-18-6	53 **I** Iodine 126.90 2-8-18-18-7	54 **Xe** Xenon 131.29 2-8-18-18-8
55 **Cs** Caesium 132.90545196 2-8-18-18-8-1	56 **Ba** Barium 137.327 2-8-18-18-8-2	57-71 Lanthanides	72 **Hf** Hafnium 178.49 2-8-18-32-10-2	73 **Ta** Tantalum 180.94788 2-8-18-32-11-2	74 **W** Tungsten 183.84 2-8-18-32-12-2	75 **Re** Rhenium 186.21 2-8-18-32-13-2	76 **Os** Osmium 190.23 2-8-18-32-14-2	77 **Ir** Iridium 192.22 2-8-18-32-15-2	78 **Pt** Platinum 195.08 2-8-18-32-17-1	79 **Au** Gold 196.97 2-8-18-32-18-1	80 **Hg** Mercury 200.59 2-8-18-32-18-2	81 **Tl** Thallium 204.38 2-8-18-32-18-3	82 **Pb** Lead 207.2 2-8-18-32-18-4	83 **Bi** Bismuth 208.98 2-8-18-32-18-5	84 **Po** Polonium (209) 2-8-18-32-18-6	85 **At** Astatine (210) 2-8-18-32-18-7	86 **Rn** Radon (222) 2-8-18-32-18-8
87 **Fr** Francium (223) 2-8-18-32-18-8-1	88 **Ra** Radium (226) 2-8-18-32-18-8-2	89-103 Actinides	104 **Rf** Rutherfordium (267) 2-8-18-32-32-10-2	105 **Db** Dubnium (268) 2-8-18-32-32-11-2	106 **Sg** Seaborgium (269) 2-8-18-32-32-12-2	107 **Bh** Bohrium (270) 2-8-18-32-32-13-2	108 **Hs** Hassium (277) 2-8-18-32-32-14-2	109 **Mt** Meitnerium (278) 2-8-18-32-32-15-2	110 **Ds** Darmstadtium (281) 2-8-18-32-32-17-1	111 **Rg** Roentgenium (282) 2-8-18-32-32-17-2	112 **Cn** Copernicium (285) 2-8-18-32-32-18-2	113 **Nh** Nihonium (286) 2-8-18-32-32-18-3	114 **Fl** Flerovium (289) 2-8-18-32-32-18-4	115 **Mc** Moscovium (290) 2-8-18-32-32-18-5	116 **Lv** Livermorium (293) 2-8-18-32-32-18-6	117 **Ts** Tennessine (294) 2-8-18-32-32-18-7	118 **Og** Oganesson (294) 2-8-18-32-32-18-8

57 **La** Lanthanum 138.91 2-8-18-18-9-2	58 **Ce** Cerium 140.12 2-8-18-19-9-2	59 **Pr** Praseodymium 140.91 2-8-18-21-8-2	60 **Nd** Neodymium 144.24 2-8-18-22-8-2	61 **Pm** Promethium (145) 2-8-18-23-8-2	62 **Sm** Samarium 150.36 2-8-18-24-8-2	63 **Eu** Europium 151.96 2-8-18-25-8-2	64 **Gd** Gadolinium 157.25 2-8-18-25-9-2	65 **Tb** Terbium 158.93 2-8-18-27-8-2	66 **Dy** Dysprosium 162.50 2-8-18-28-8-2	67 **Ho** Holmiun 164.93 2-8-18-29-8-2	68 **Er** Erbium 167.26 2-8-18-30-8-2	69 **Tm** Thulium 168.93 2-8-18-31-8-2	70 **Yb** Ytterbium 173.05 2-8-18-32-8-2	71 **Lu** Lutetium 174.97 2-8-18-32-9-2
89 **Ac** Actinium (227) 2-8-18-32-18-9-2	90 **Th** Thorium 232.04 2-8-18-32-18-10-2	91 **Pa** Protactinium 231.04 2-8-18-32-20-9-2	92 **U** Uranium 238.03 2-8-18-32-21-9-2	93 **Np** Neptunium (237) 2-8-18-32-22-9-2	94 **Pu** Plutonium (244) 2-8-18-32-24-8-2	95 **Am** Americium (243) 2-8-18-32-25-8-2	96 **Cm** Curium (247) 2-8-18-32-25-9-2	97 **Bk** Berkelium (247) 2-8-18-32-27-8-2	98 **Cf** Californium (251) 2-8-18-32-28-8-2	99 **Es** Einsteinium (252) 2-8-18-32-29-8-2	100 **Fm** Fermium (257) 2-8-18-32-30-8-2	101 **Md** Mendelevium (258) 2-8-18-32-31-8-2	102 **No** Nobelium (259) 2-8-18-32-32-8-2	103 **Lr** Lawrencium (266) 2-8-18-32-32-8-3

exception
v.e = 2
should be
g2
but its properities are alike with
g8

noble gases:
their last shell is Full of e^- thats why they are stable
they don't give, recieve or give e^-

لهم القدرة
لأنهم منتهين من
الوصول للاستقرار

* unstable elements tend to build chemical bonds to reach stability .....

- **Chemical Bonds**

occurs between metals & non metals

1. Ionic Bonding

(رابطة أيونية)

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

(complete transfer of e$^-$ from one element to another)

ex: NaCl

$s^2\ s^2\ p^6\ s^1$ –

$$^{11}\text{Na} : [\text{Ne}]\,3s^1 \xrightarrow{-e} \overset{\oplus}{\text{Na}} : [\text{Ne}]$$

easier to lose one e$^-$ to become like (Ne) (rather to receive 7) and become like (Ar)

$s^2\ s^2\ p^6\ s^2\ p^5$

$$^{17}\text{Cl}: [\text{Ne}]\,3s^1\,3p^5 \xrightarrow{+e} \text{Cl}^{\ominus} : [\text{Ar}]$$

easier to receive one e$^-$ to become like (Ar) rather than giving up 7 to become like (Ne)

ex: Na-Cl

look at (توزيع e$^-$) in the periodic table

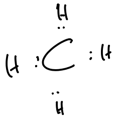
The resulting e$^-$ configuration of both ions are those of the nearest noble gas, Ne and Ar respectively, both satisfy the octet rule.

↳ last shell having 8e$^-$ (full)

2. Covalent Bonding

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

* (there are two types of covalent Bonds) ⇝ (polar / non polar)
① ②



$\boxed{\text{or}}$

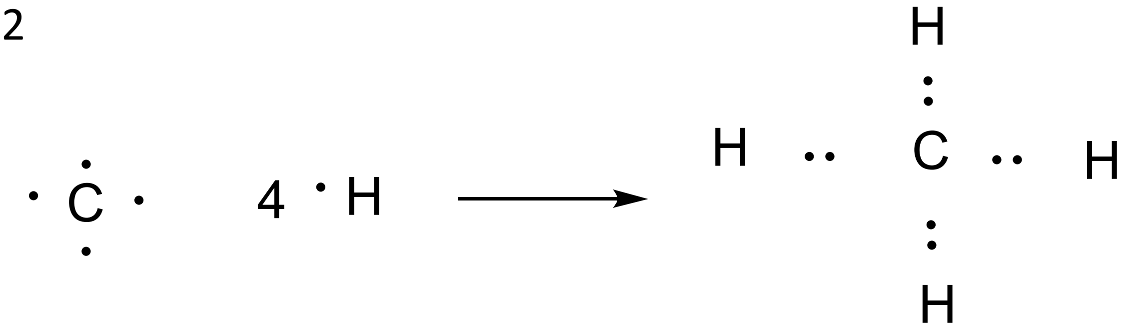
$2\,\mathrm{H}\cdot \longrightarrow \boxed{\mathrm{H}{:}\mathrm{H}}$

last shell full of e^- → stable

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



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

مدى حب الذرة للالكترون

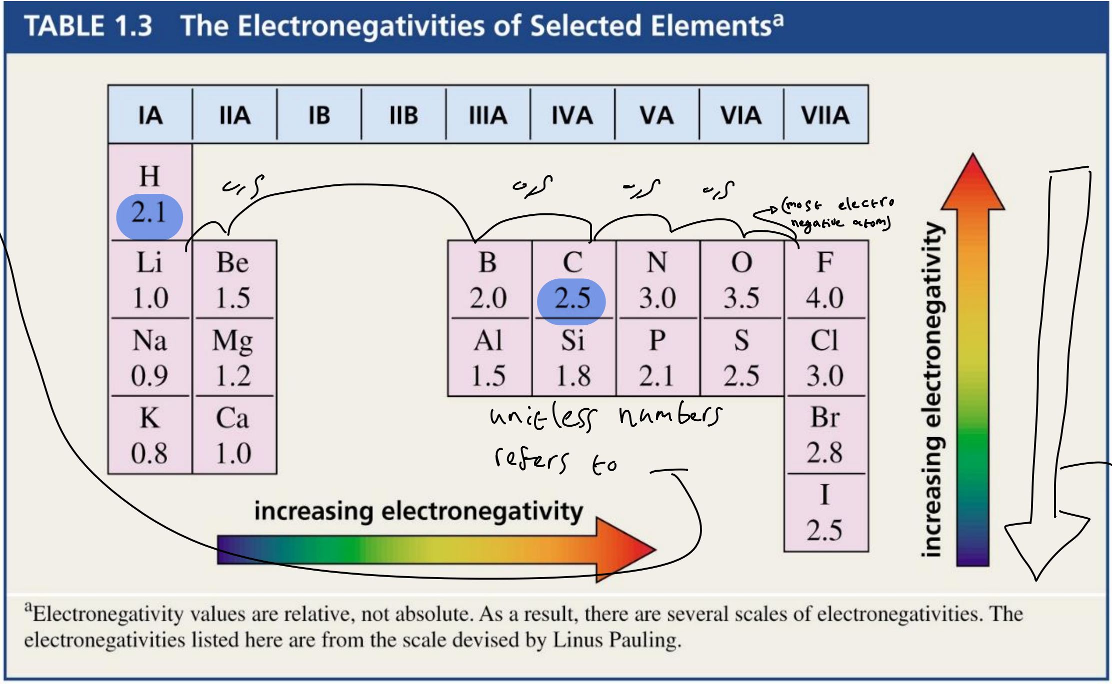


TABLE 1.3 The Electronegativities of Selected Elements[a]

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

increasing electronegativity

increasing electronegativity

[a] Electronegativity 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.

[illegible] [illegible] [illegible] [illegible]

(most electro negative atom)

unitless numbers

refers to

close to nucleus (strong attraction)

covalent bond

size of atom increases

far from nucleus (weak attraction)

Covalent bonds can be classified as

A. Nonpolar covalent bond (Δ EN = 0-0.5)

Examples C-C C-H

ΔEN = 0 ΔEN = 0,4

normally in covalent bond 2e⁻ are in the middle

A—B

covalent bond

if A has more electro negativity,

Polarization will happen (e⁻ density will be more around A so it will be partially negative)

$\overset{-\delta}{A}-\overset{+\delta}{B}$

A:⊂⊃B

Polarization

B. Polar covalent bond (Δ EN = 0.5 1.9)

O–H
1,4

N – H
0,9

A polar bond has a negative end and a positive end (polarized)

dipole moment (D) = μ = *e* x *d*

(*e*) : magnitude of the charge on the atom (كمية ال charge)

(*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 Δ EN increases the polarity increases

μ increases

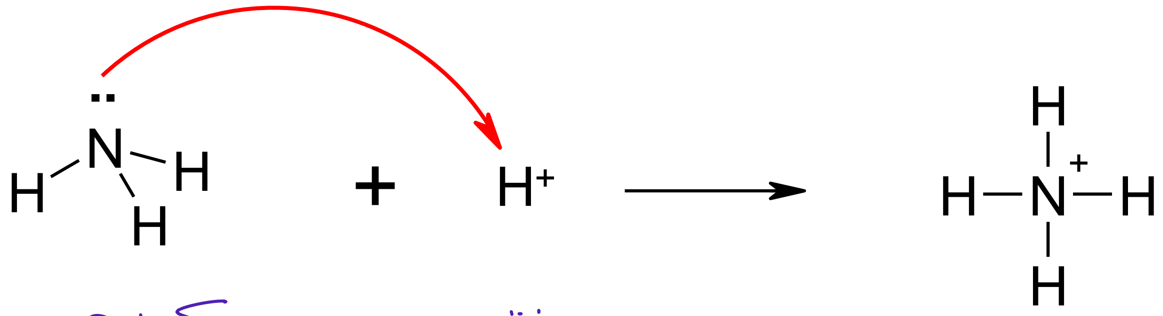
Note : If Δ EN is more than 1.9then the bond is ionic Ex: Li-F

not covalent anymore !!!

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.

$$NH_3 + H^+ \rightarrow NH_4^+$$



كريم فقير

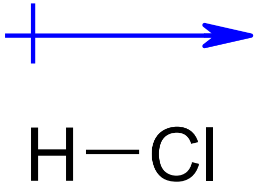
كريم shares with فقير

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.

permanent and partial

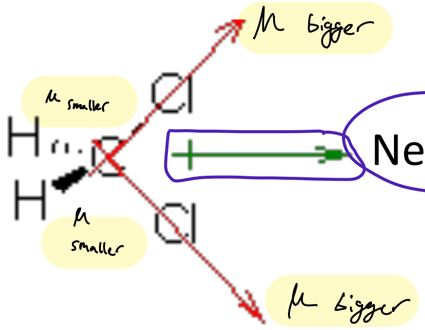
$$\overset{\delta^+}{\text{H}}-\overset{\delta^-}{\text{Cl}}$$



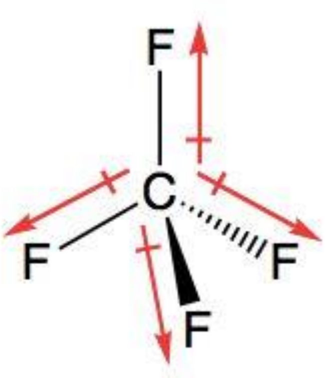
Bond Polarity & Electronegativity (cont'd)

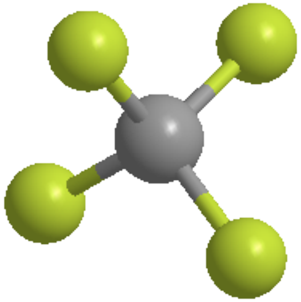
⊕ the more ΔEN

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



Net dipole moment ≠ 0





Net dipole moment =0

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).

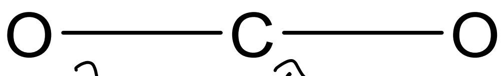
CO_2= 4+2(6) =16.

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. (not central) *

H

Cl/I/Br/F

(طرفي)



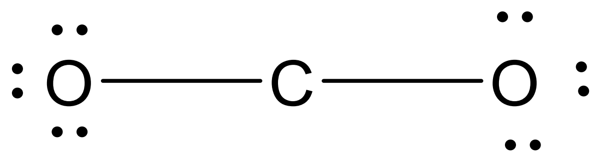
3) determine number of remaining e^-. complete the octet of the terminal atoms.

(after drawing bonds)

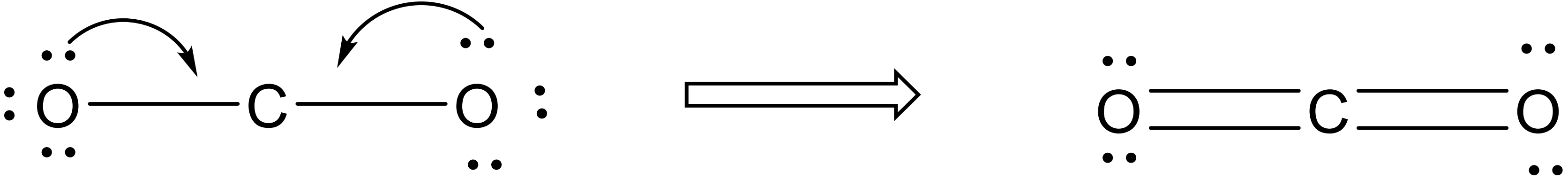
8e⁻ around every atom for stability

(full e⁻ in last shell)

16 -4 = 12



4) Complete the octet Use lone pair e$^-$ from terminal atoms to create multiple bonds. so the central atom achieves the octet rule



5) determine the formal charges of all atoms.

CO$_2$ is neutral

$\boxed{\Sigma \text{formal charge} = 0}$

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

formal charge = [VE − (dots + dashes)]

For O $6-\overset{(4+2)}{6}=0$

For C 4-4 =0

لازم zero

Ex: NO_3^-

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

recieved e^-

$6-(4+2)=\boxed{0}$

O = $6-(6+1) = \boxed{-1}$

Formal charge

$= \boxed{-1 = -1}$ ✓

N = $5-(0+4)=\boxed{+1}$ ✓

$24 - 3*2 = 18/3 = \underline{6\text{ dots}}$

N (7) O (8)

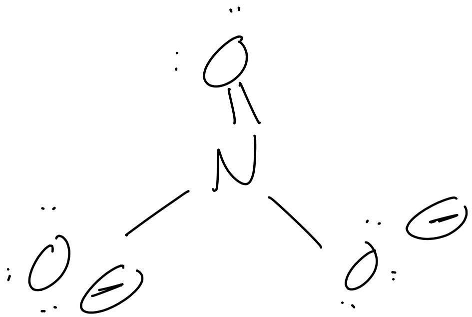
$s^2\ s^2\ p^3$

ve=5

$s^2\ s^2\ p^4$

ve=6

$\Sigma Ve = 5+18+1=\boxed{24}$



$6-(4+2)=0$

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

$5-4=+1$

$-1-1+1+0=\boxed{-1}$

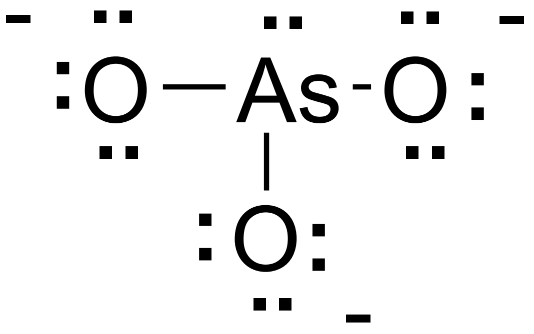
*

Correct

Lewis Structures (other examples)

Example 2: AsO_3^{3-}

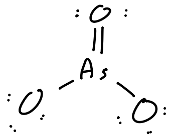
1) # e^-: $5 + 3(6) + 3 = 26$
2) form 3 single bonds
3) 20 e^- remain
4) O needs 6, As needs 2
5) All octets
6) Formal charges



As 2-8-18-5

$18 + 5 + 3 = \boxed{26}$

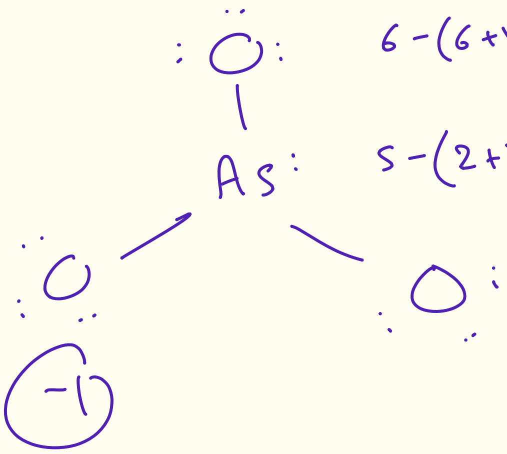
O 2-6



AsO_3^{-3}

(5) (6)

$\Sigma Ve = 5 + 18 + 3 = \underline{\underline{26}}$



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

$5 - (2+3) = 0$

-1

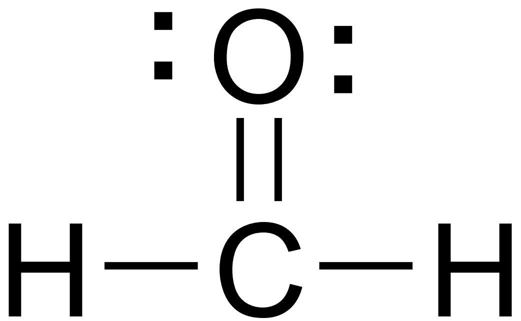
$-1 + -1 + -1 = \boxed{-3}$

✓

Lewis Structures (cont’d)

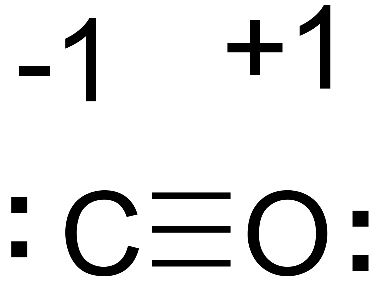
Example 3: CH_2O

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



Lewis Structures (cont’d)

Example 4: CO



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

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

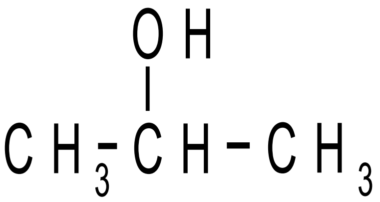
1.8 Isomers

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

They have different physical and chemical properties:

$CH_3-CH_2-CH_2-O-H$

1-propanol
(bp 97.4 C)



$CH_3-\overset{\overset{\displaystyle OH}{|}}{C}H-CH_3$

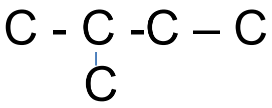
2-propanol
(bp 82.4 C)

1.9 Writing Structural Formulas

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

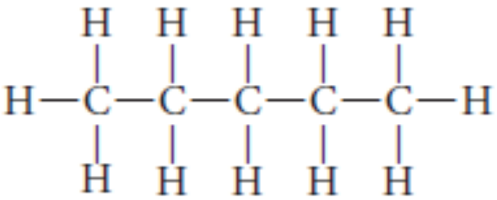
C - C - C -C - C

Continuous chain

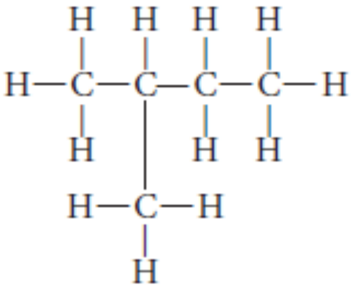


$$\mathrm{C - \underset{\underset{\displaystyle C}{|}}{C} - C - C}$$

Branched chain



pentane, bp 36°C



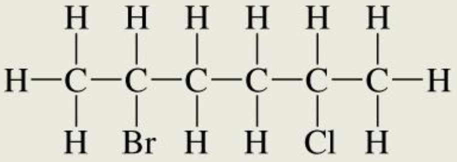
2-methylbutane, bp 28°C
(isopentane)

C forms 4 covalent bonds

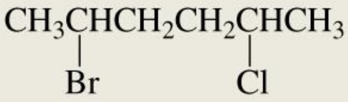
Dash formula

Kekulé structure **Condensed structures** **Bond line formula**

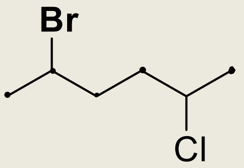
Atoms bonded to a carbon are shown to the right of the carbon. Atoms other than H can be shown hanging from the carbon.



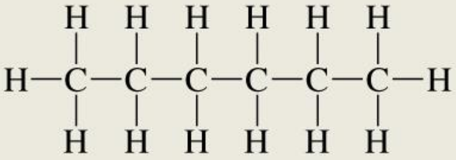
~~or~~ $CH_3CHBrCH_2CH_2CHClCH_3$ or



$CH_3\underset{Br}{C}HCH_2CH_2\underset{Cl}{C}HCH_3$ ~~or~~

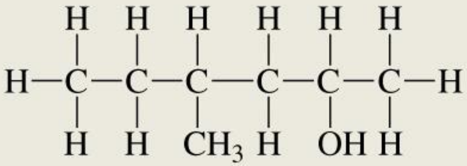


Repeating CH_2 groups can be shown in parentheses.

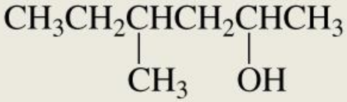


$CH_3CH_2CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_4CH_3$

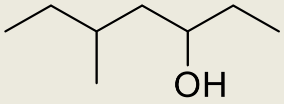
Groups bonded to a carbon can be shown (in parentheses) to the right of the carbon, or hanging from the carbon.



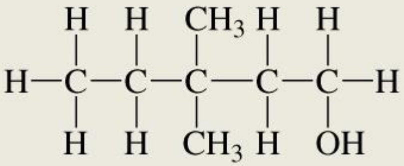
$CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$ or



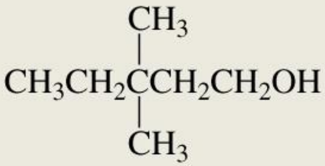
$CH_3CH_2\underset{CH_3}{C}HCH_2\underset{OH}{C}HCH_3$



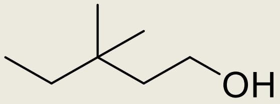
Groups bonded to the far-right carbon are not put in parentheses.



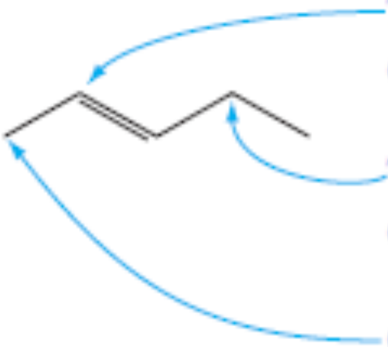
$CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or



$CH_3CH_2\overset{CH_3}{\underset{CH_3}{C}}CH_2CH_2OH$



$CH_3CH{=}CHCH_2CH_3$

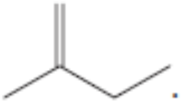


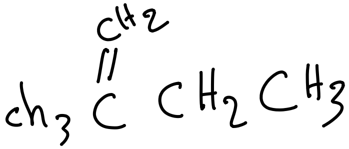
Three line segments emanate from this point; therefore, this carbon has one hydrogen (4 − 3 = 1) attached to it.

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.

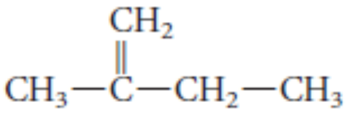
EXAMPLE 1.12

Write a more detailed structural formula for .



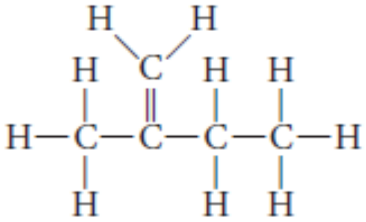
$$ch_3\overset{CH_2}{\overset{\|}{C}}CH_2CH_3$$

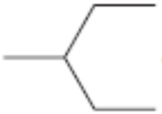
Solution

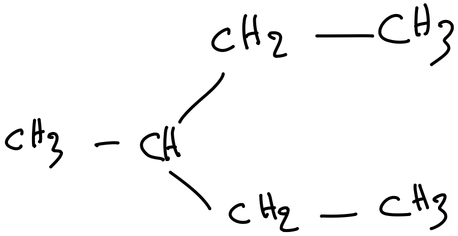


$$CH_3-\overset{CH_2}{\overset{\|}{C}}-CH_2-CH_3$$

or



PROBLEM 1.23 Write a more detailed structural formula for .

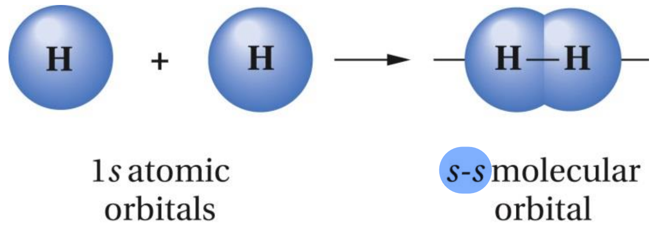


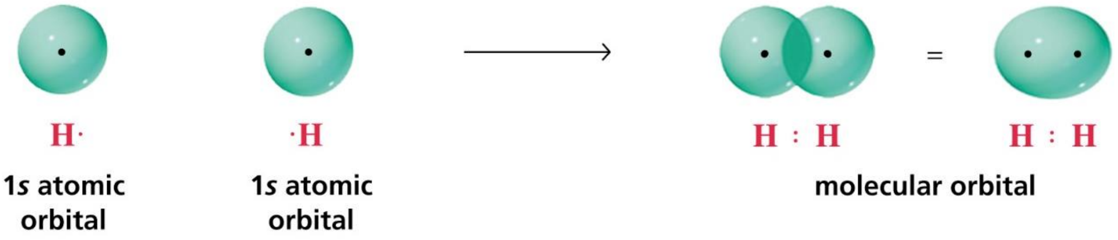
1.14 The Orbital View of Bonding; the Sigma Bond

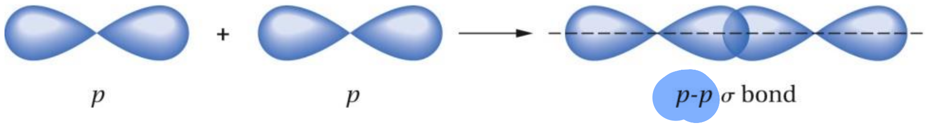
(covalent)

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

when covalent bonds are about to form between atoms orbitals approach each other in specific ways.







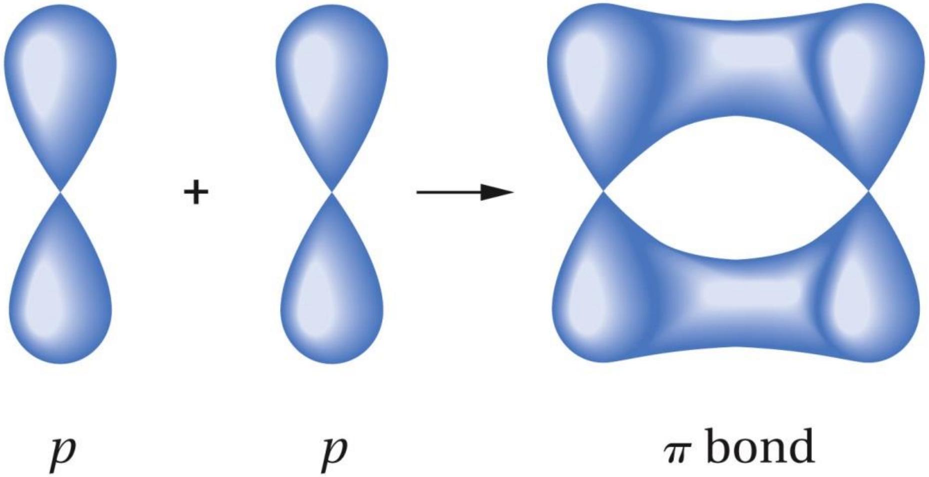
Orbitals approach each other in a **head to head** fashion ⇝ sigma bond s-s or p-s or p-p

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

[happens when (only) p - p orbitals approach each other side ways.]

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

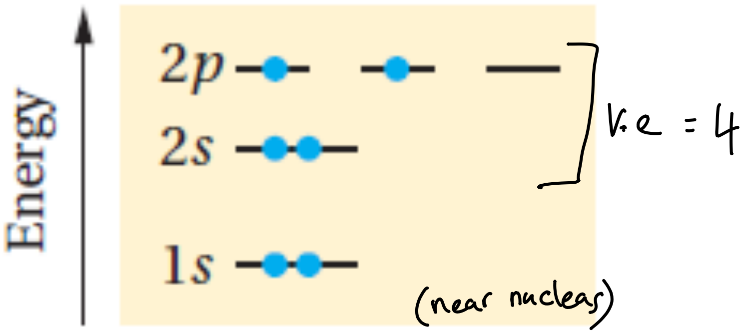


parallel to each other

Carbon sp^3 Hybrid Orbitals

(Hybridization)

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

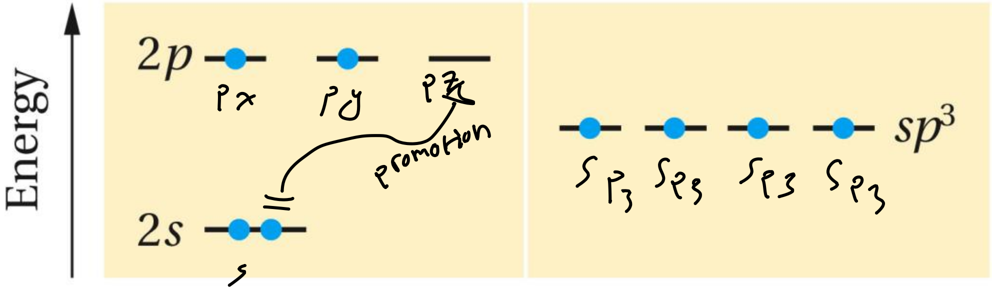


Distribution of the six electrons in a carbon atom. Each dot stands for an electron.

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

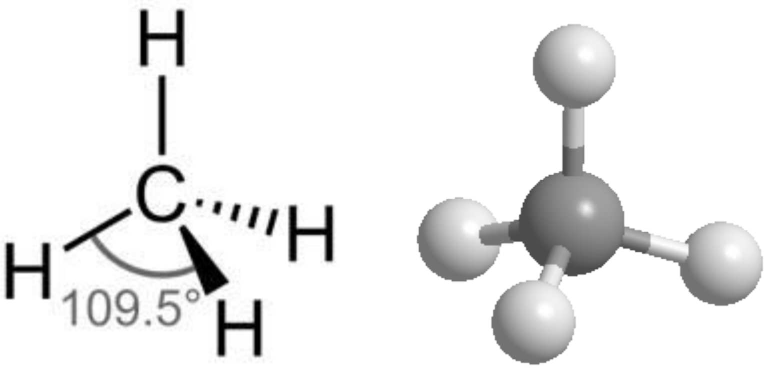
A: We know from experience that carbon usually forms *four* single bonds, and often these bonds are all equivalent, as in CH_4

(s mixes with 3 p for equivalence)



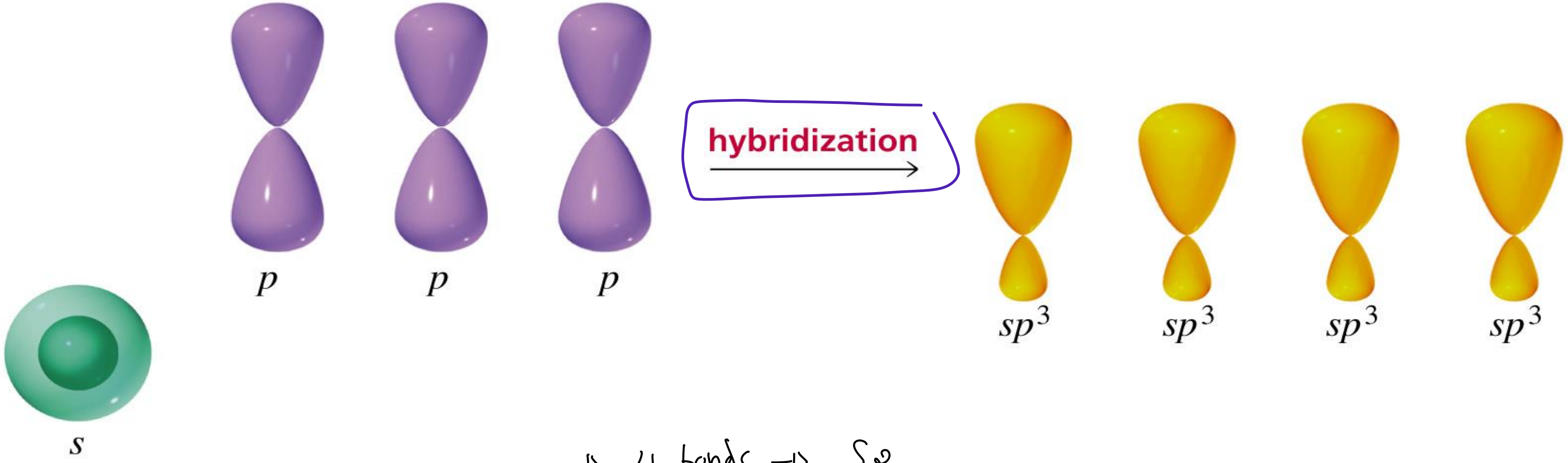
Atomic orbitals of carbon

Four equivalent sp^3 hybrid orbitals

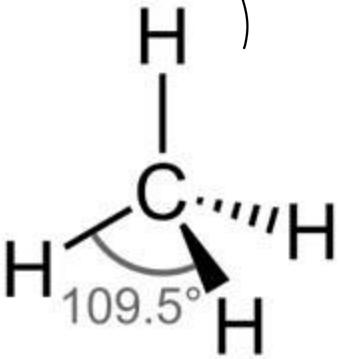


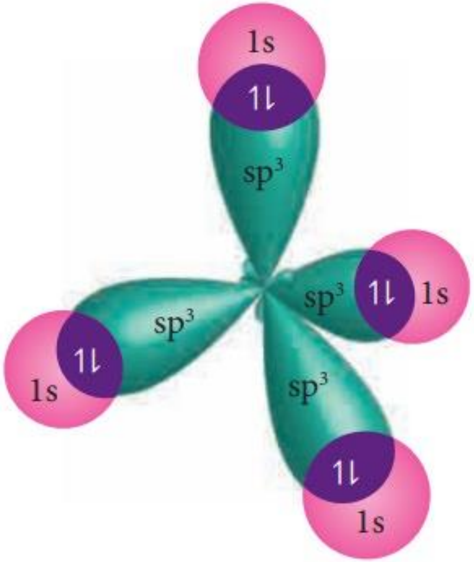
3D Structure of Methane Molecule

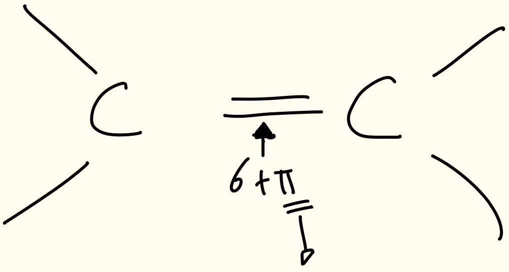
Mix or combine the four atomic orbitals of the valence shell to form four identical hybrid orbitals



→ 4 bonds → Sp_3



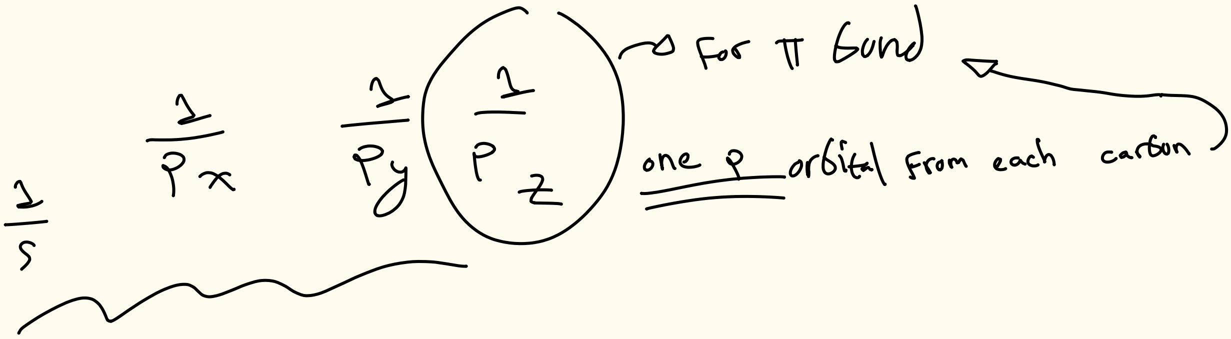




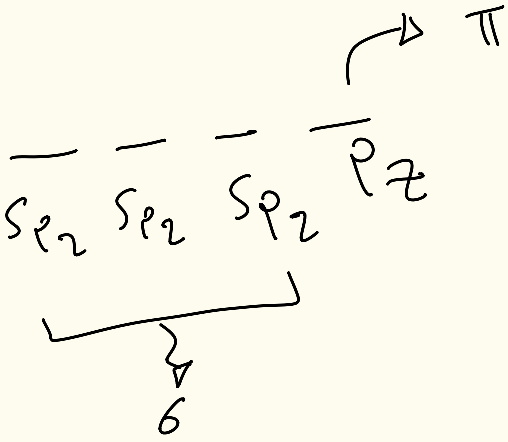
p + p

(side to side)

each p is from each carbon



For σ sigma

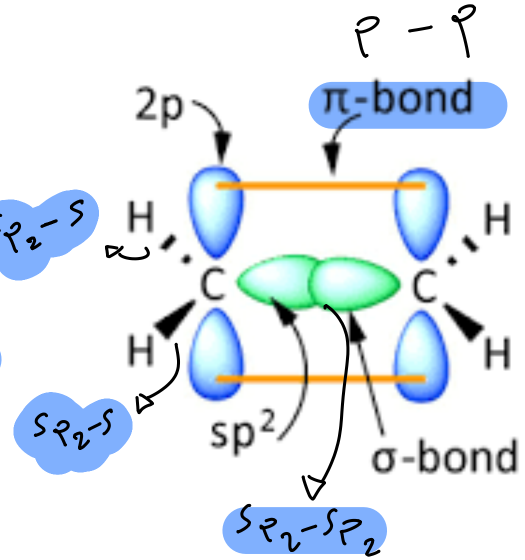


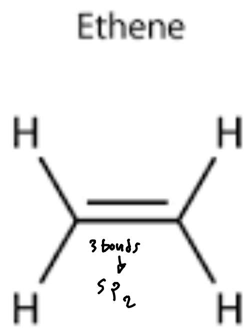
SP^2-Hybridized orbitals

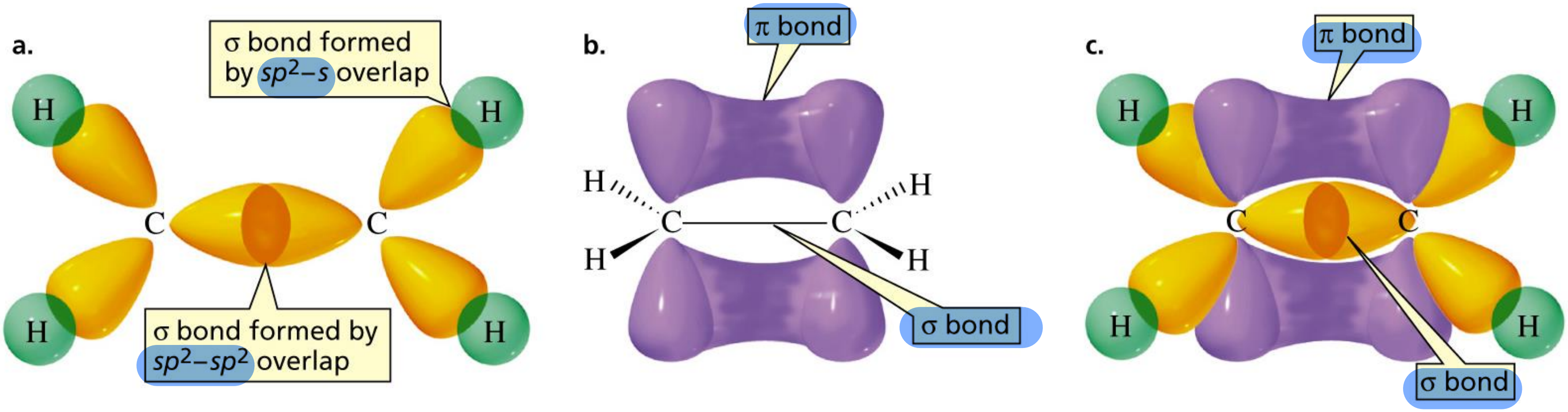
One part *s* and two parts *p* in character and are directed toward the three vertices of an equilateral triangle.

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.



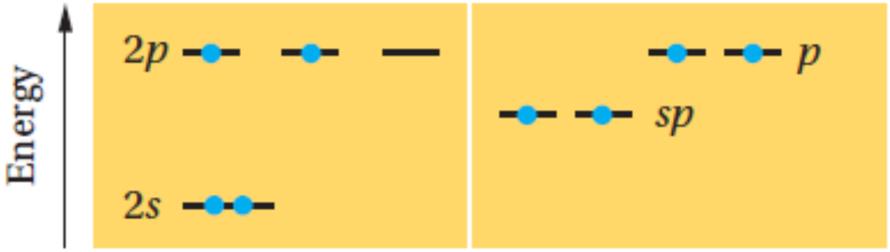




SP-Hybridized orbitals

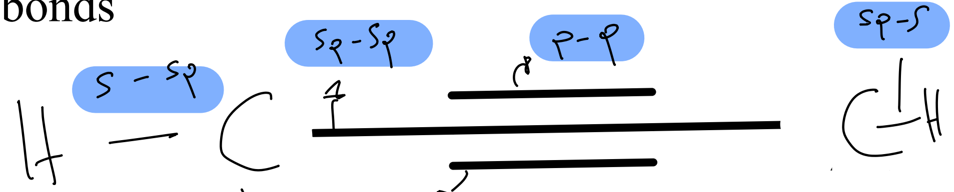
Bonding in Ethyne: **A Triple Bond**

- 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.



4 bonds

two σ

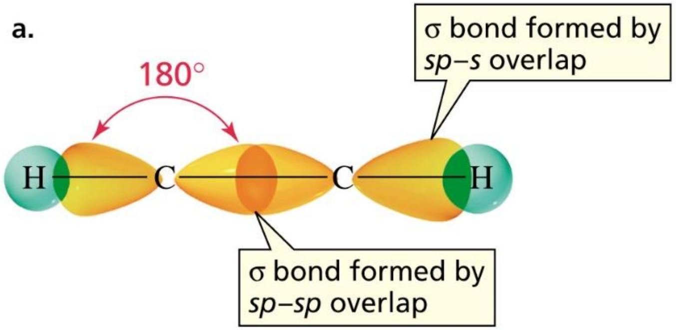
sp

σ + 2π

2p orbitals from each carbon

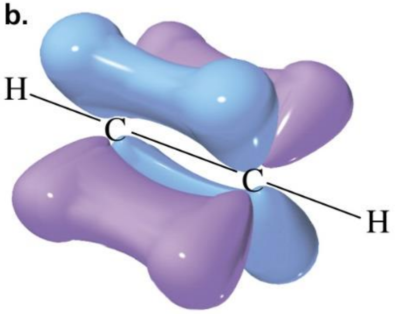
ex: H - Ö - H → sp

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



σ bond formed by *sp*–*s* overlap

σ bond formed by *sp*–*sp* overlap



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

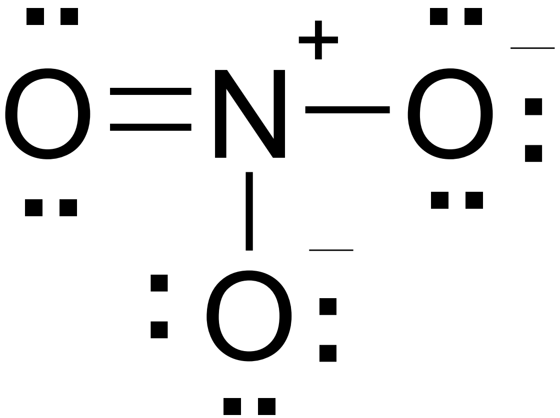
There are molecules (or ions) for which more than one correct Lewis structure can be drawn, these equivalent Lewis structures are resonance structures.

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 chargall es

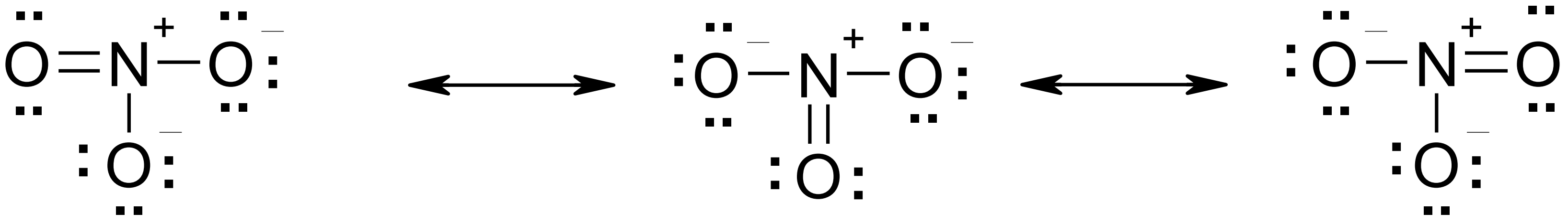
(=) is shorter than (−)

Resonance (cont'd)

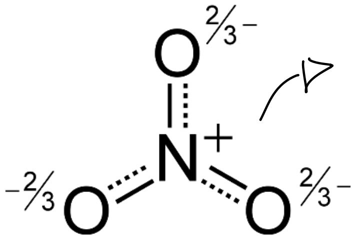
Example 1: NO_3^- (cont'd)

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 and C are resonance structure (they only differ in e^- positions) (bond position)



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



A **resonance hybrid**

same charges

same bond length

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

the e⁻ that are changed in position are either

Rules for drawing resonance structures :

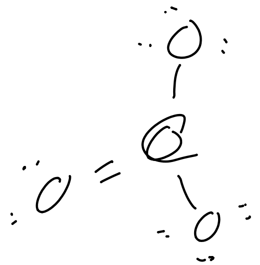
1) Electrons only can be moved (lone pair / π electrons)

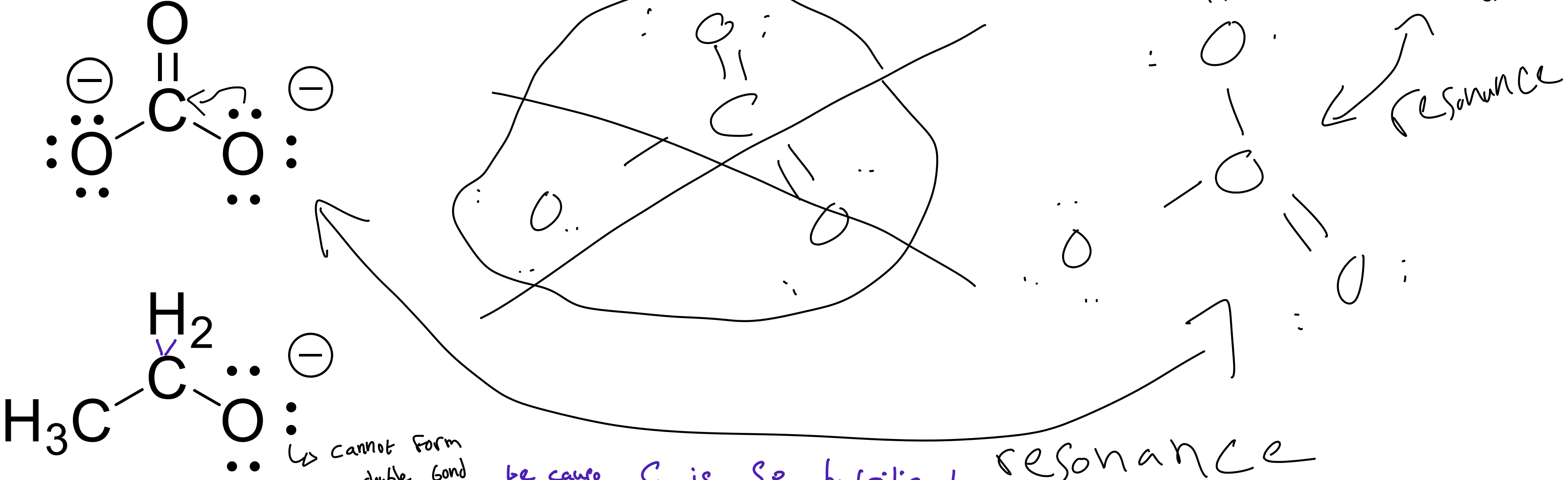
(= / ≡)

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

(not sp3)

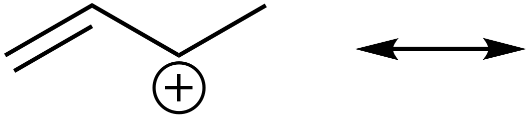
Examples: Write a second resonance structure for the following compounds?





↳ cannot form double bond because C is sp_3 hybridized atom

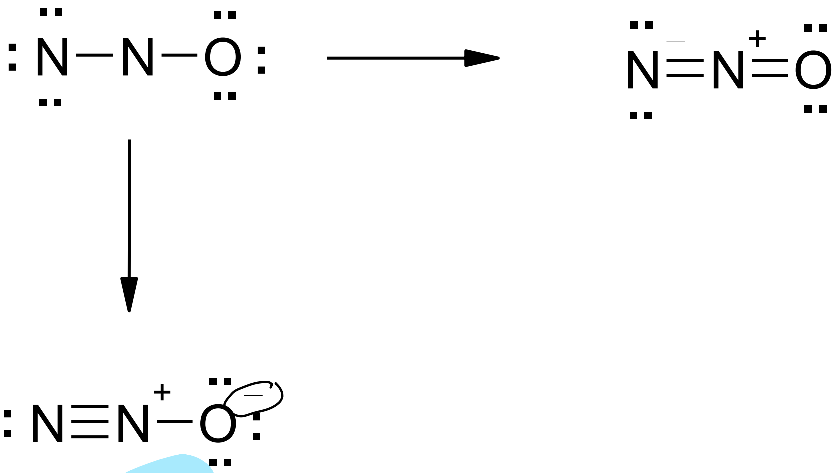
Exercise



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?



because O is more EN

so it's more stable

N_2O $\Sigma ve = 10 + 6 = 16e^-$

$16 - 4 = 12e^-$

$:\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}} — N — \underset{\cdot\cdot}{\overset{\cdot\cdot}{O}}:$

$5-(6+1) = -2$ $+1$ $6-(2+3) = +1$

$:\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}} - N \equiv O^{\cdot\cdot}$

$5-(2+5 = 0$ $5-(4) = \boxed{+1}$ $6-(6+1) = \boxed{-1}$

✓ ⊛ $:N \equiv N - \underset{\cdot\cdot}{\overset{\cdot\cdot}{O}}:$

$5-4 = \boxed{+1}$

$:\ddot{N} = N = \underset{\cdot\cdot}{O}:$ $6-(4+2) = 0$

$5-(4+2) = \boxed{-1}$

a

Classification of organic compounds

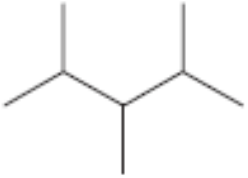
1.17: Classification According to Molecular Framework

(الشكل)

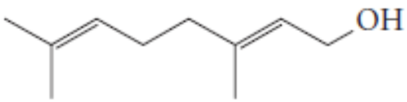
- The three main classes of molecular frameworks for organic structures are **acyclic**, **carbocyclic**, and **heterocyclic** compounds.

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

unbranched chain of eight carbon atoms



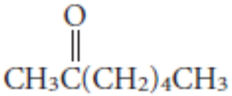
branched chain of eight carbon atoms



geraniol
(oil of roses)
bp 229–230°C

$CH_3(CH_2)_5CH_3$

heptane
(petroleum)
bp 98.4°C

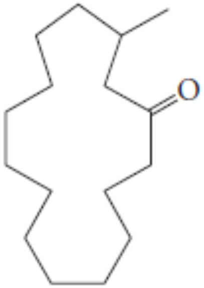


$CH_3\overset{\overset{\displaystyle O}{\|}}{C}(CH_2)_4CH_3$

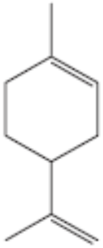
2-heptanone
(oil of cloves)
bp 151.5°C

1.17b: Carbocyclic Compounds: contain rings of carbon atoms

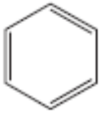
carbon forms the rings



muscone
(musk deer)
bp 327–330°C



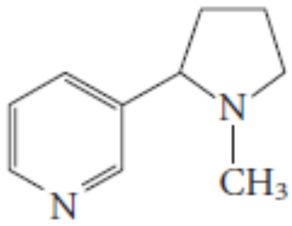
limonene
(citrus fruit oils)
bp 178°C

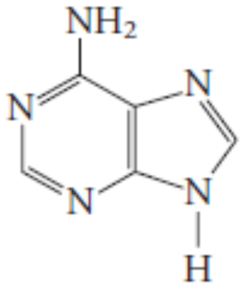


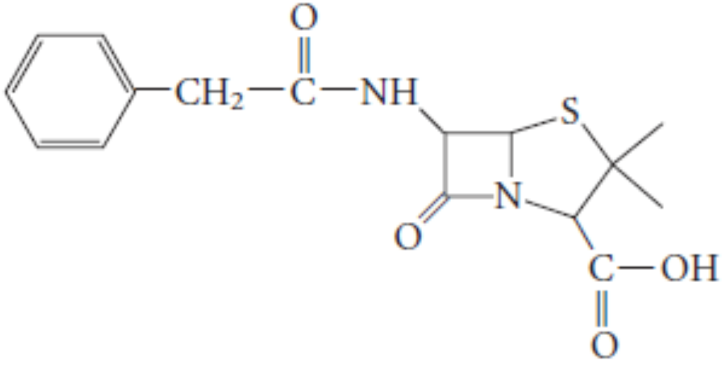
benzene
(petroleum)
mp 5.5°C, bp 80.1°C

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...)

(atleast one atom replaces one carbon in the ring)


nicotine
bp 246°C


adenine
mp 360–365°C
(decomposes)


penicillin-G
(amorphous solid)

{B}

Classification According to Functional Group (more accurate)

A functional group is an arrangement of atoms with distinctive **physical** and **chemical** properties. (molecules that share the same functional group are alike in some properities.)

C–C–OH

$C-C-\overset{OH}{C}-C$

Table 1.6 ▰ The Main Functional Groups

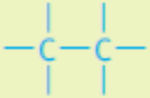
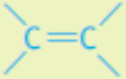
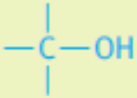
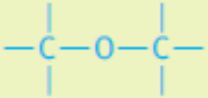
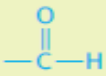
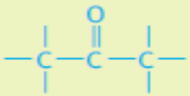
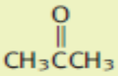
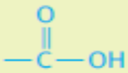
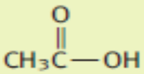
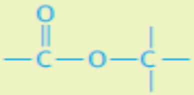
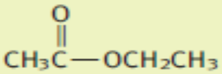
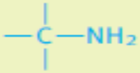
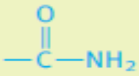
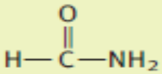
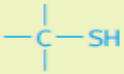
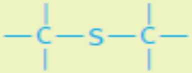
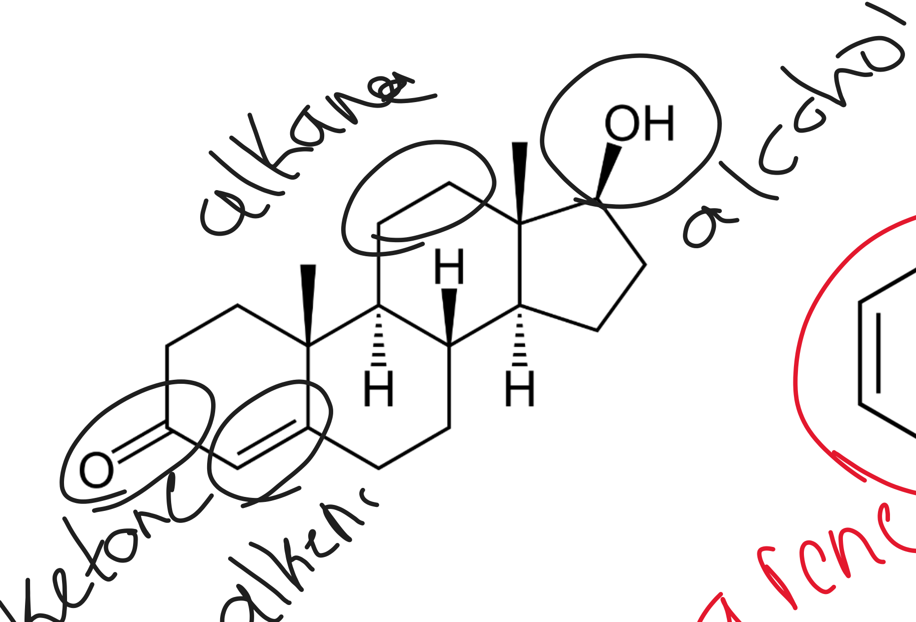
	Structure	Class of compound	Specific example	Common name of the specific example
A. Functional groups that are a part of the molecular framework	 $-\overset{\vert}{\underset{\vert}{C}}-\overset{\vert}{\underset{\vert}{C}}-$	alkane	$CH_3—CH_3$	ethane, a component of natural gas
		alkene	$CH_2=CH_2$	ethylene, 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	 $-\overset{\vert}{\underset{\vert}{C}}-OH$	alcohol	CH_3CH_2OH	ethyl alcohol, found in beer, wines, and liquors
	 $-\overset{\vert}{\underset{\vert}{C}}-O-\overset{\vert}{\underset{\vert}{C}}-$	ether	$CH_3CH_2OCH_2CH_3$	diethyl ether, once a common anesthetic

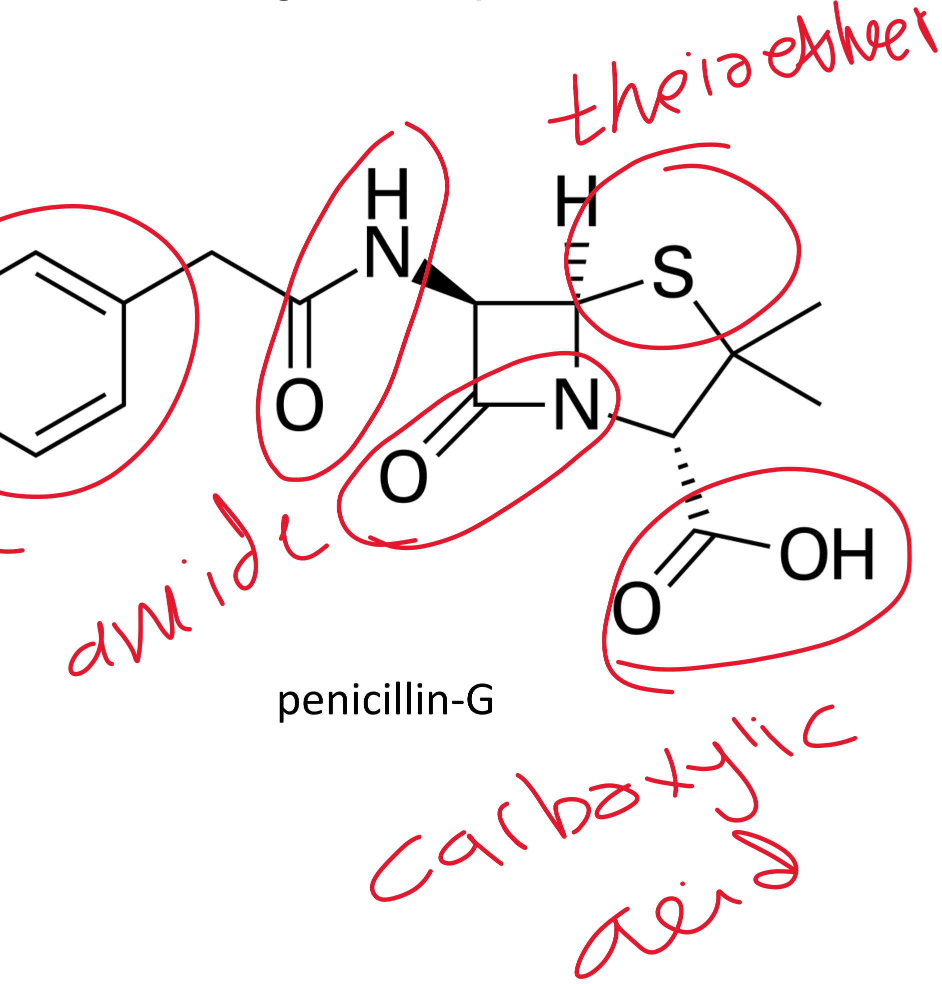
Table 1.6 — continued

	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 (cl Br I f)	$-X$	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