

MOHAMED KHIDER UNIVERSITY OF BISKRA.
FACULTY OF EXACT SCIENCES AND NATURAL AND LIFE SCIENCES
DEPARTMENT OF BIOLOGY

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Dr: Ismail DAOUD

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1.5. Chemical bond

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1.5. Chemical bond

1.5.1. Introduction: strong bonds and weak bonds

In this section, we will try to answer the fundamental questions:

- Why do some atoms form a molecule while others do not?
- Why are some molecules linear while others are not?

Answer:

⇒ The bond does not affect the deep shells of atoms, only the electrons of the last shell or peripheral (or valence) shell will be engaged to form the bond (molecule).

⇒ The molecule will only exist if its total energy is lower than that of separate atoms, that is, the molecule obtained must be more stable than the atoms they make formed.

After learning how the elements are arranged in the periodic table, we will focus on forming the bonds between these elements.

1.5.2. Different types of strong bonds (covalent bond, ionic bond, dative bond...)

We distinguish:

1. Bonds between atoms: Strong bonds: Ionic bond, Covalent bond, dative bond, and metal bond.

2. Bonds between molecules: These are weak bonds: H-bond (Hydrogen bond), Hydrophobic bonds, Steric bonds,....etc.

1.5.2. Different types of strong bonds

We will treat respectively the covalent (The polarized covalent bond, the unpolarized covalent bond), ionic bond and finally dative bond.

It should be noted that the nature of the bonds depends on the electro-negativity of the atoms.

a. The covalent bond

The unpolarized covalent bond (U.C.B):

In the covalent bond, each atom shares 1 electron, the bond is distributed equally between the two atoms concerned.

If these atoms are identical, the molecule formed will be homo-nuclear (H_2 , O_2 , Cl_2 , etc.).

The covalent bond is non-polar (of the same polarity).

The polarized covalent bond(P.C.B):

If these atoms are different, the molecule will be hetero-nuclear (NH_3 , CH_4 , C_2H_4 , etc.).

In the hetero-nuclear molecule, there is some difference in electro-negativity between atoms; the covalent bond formed will be polarized covalent (polarized covalent bond).

Note:

The more the number of covalent bonds between two atoms increases, the more the bond length(distance) decreases and thus the bond energy increases and the bond becomes stronger (case of the passage from C-C to C=C and C \equiv C).

The bonds formed can be single or multiple:

Difluor: $\text{F}_2 \Rightarrow \text{F-F}$: Single link 1 doublet σ .

Oxygen: $\text{O}_2 \Rightarrow \text{O=O}$: Double bond 1 doublet σ and 1 doublet π .

Diazote: $\text{N}_2 \Rightarrow \text{N}\equiv\text{N}$: Triple 1 doublet σ and 2 doublet π .

a. The dative bond (D.B):

It happens that a molecule is formed from two atoms, one of which has a free doublet (a pair of electrons) and the other, empty quanta box (a gap).

The link of this doublet constitutes a dative bond (NH_4^+ , H_3O^+ , OH^- , ... etc.).

b. The ion bond (I.B):

When we are in the presence of two atoms whose difference of electro-negativity important, there is no common of the electron but there is a «transfer» of this electron, from the least electronegative atom to the most electronegative atom and an ion bond is thus formed. This bond is provided by forces of electrostatic origin. Such bonds give rise to ionic compounds.

Example:

Na^+Cl^- : this type of bond usually occurs between elements of groups IA, IIA and elements of groups VIA, VIIA.

1.5.3. Representation of the chemical bond: Lewis diagram

a. Lewis Theory:

In 1916 Gilbert N. Lewis was led to consider the covalent bond as resulting from the sharing of one or more electron pairs.

b. Lewis representation of atoms and molecules:

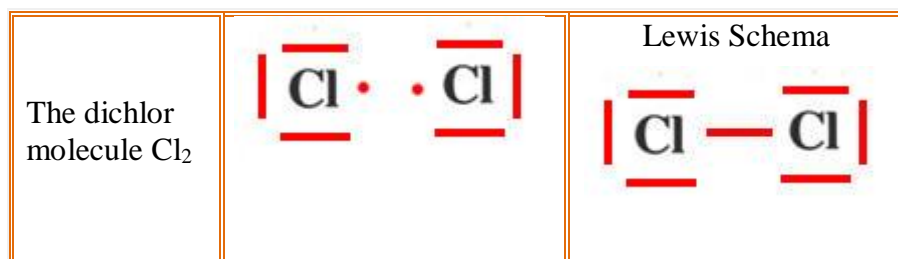
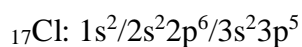
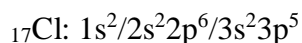
Lewis' representation schematizes the external electronic structure of an atom, also known as the valence shell.

- Paired electrons are represented by dashes: —
- Single electrons are represented by dots: •
- No electrons are represented by: Vacant box (empty) ☐

Rules:

This representation of the molecule is based on the octet rule (from the Greek: eight (8) i.e. each atom surrounded by eight electrons)

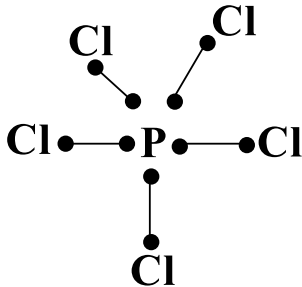
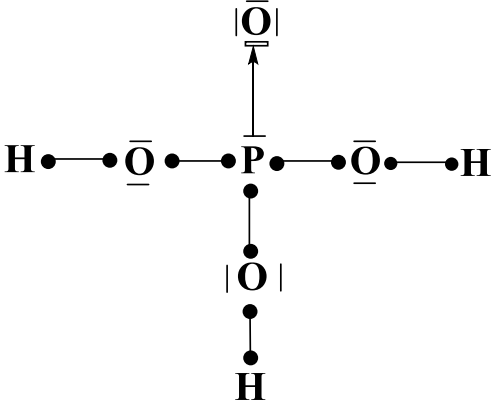
Example: Cl₂



c. Valence of an atom and exceptional case (excitation)

The valence most often corresponds to the number of single electrons present in the valence shell of the element studied.

The valence of an atom can be modified by using excited levels.

<u>Increase valence:</u> move electrons forward (Example: PCl ₅).	<u>Decrease valence:</u> move electrons backwards (Example: H ₃ PO ₄).
<u>Exemple :</u> PCl ₅ $_{15}\text{P}: 1s^2/2s^22p^6/3s^23p^3/3d^0 \Rightarrow$ $_{15}\text{P}: 1s^2/2s^22p^6/3s^13p^3/3d^1$ $_{17}\text{Cl}: 1s^2/2s^22p^6/3s^23p^5$ 	<u>Exemple :</u> H ₃ PO ₄ $_{1}\text{H}: 1s^1 \Rightarrow$ $_{15}\text{P}: 1s^2/2s^22p^6/3s^23p^3$ $_{8}\text{O}: 1s^2/2s^22p^4$ $_{8}\text{O}: 1s^2/2s^22p^4$ $_{8}\text{O}: 1s^2/2s^22p^4$ $_{8}\text{O}: 1s^2/2s^22p^4$ 

1.5.4. Geometry of molecules: V.S.E.P.R theory (Gillespie's rule)

a. Principle of the method

In many cases, the geometric shape of molecular buildings can be obtained from Gillespie's rules, known as VSEPR ("Valence Shell Electron Pair Repulsion")

Gillespie's rules are based on electrostatic data. If we have an atom A, all binding or nonbinding electronic pairs (and possibly single electrons) are arranged to minimize electrostatic repulsions.

b. Using the VSPER method to determine the type of molecule

Global geometry of the molecule:

We have a general write: AX_mEn

A: central atom;

m: the number of binding doublets (who participate in the bond)

n: the number of non-bonded doublets (who do not participate in the bond).

m+n: the total number of doublets

How do you choose the central atom?

Condition 1: Choose the atom with the smallest stoichiometric coefficient. If not, proceed to the second condition.

Condition 2: Choose the atom with the highest number of single electrons. If not, proceed to the third condition.

Condition 3: Choose with the highest atomic number Z.

Example: NH_3

The central atom is N (Choice of the central atom according to the 1st condition)

The bound atom is H, with $m=3$ binding doublets X_3 .

The N atom in this molecule has 1 free doublet ($n=1$)

$E_n = E$.

Global geometry of the NH_3 is: AX_3E .

Important note :

If the molecule has multiple bonds (double π or triple σ, π), each bond will be considered simple (σ bond).

$\text{C}=\text{C}$ 2 single bonds 1 doublet binder.

$\text{C}\equiv\text{C}$ 3 single bonds 1 doublet binder.

Example: C_2H_4

$\text{H}_2\text{C}=\text{CH}_2$

The central atom is $\text{C} \Rightarrow \text{A}$

The atom C is bound with two H and one C, with $m=3$ binding doublets X_3 .

$n=0$ (no free doublets) $E_n = E_0=0$.

Global geometry of the C_2H_4 is: AX_3 .

Hybridization types:

In general, to know the hybridization of a molecule from its AX_mE_n geometry, the procedure is as follows:

If: $m+n=2$ Hybridization of an atomic orbital (OA) "S" and an atomic orbital "p" Hybridization Sp .


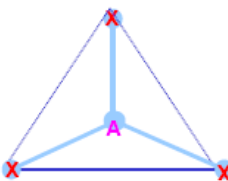
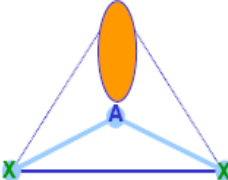
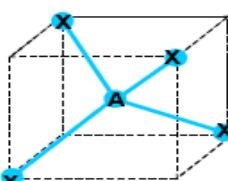
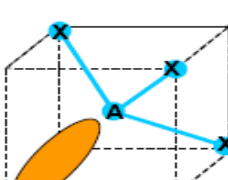
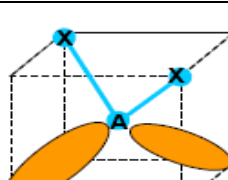
If: $m+n=3$ Hybridization of an atomic orbital (OA) "S" and two atomic orbitals "p" Hybridization Sp^2 .

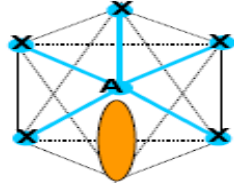
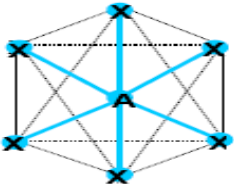
If: $m+n=4$ Hybridization of an atomic orbital (OA) "S" and three atomic orbitals "p" Hybridization Sp^3 .

If: $m+n=5$ Hybridization of an atomic orbital (OA) "S" and three atomic orbitals "p" and an atomic orbital "d" Hybridization Sp^3d .

If: $m+n=6$ Hybridization of an atomic orbital (OA) "S" and three atomic orbitals "p" and two atomic orbitals "d" Hybridization Sp^3d^2 .

Specific geometry to the molecule:**Table:** Prediction of the geometry of molecules according to the VSEPR method (Gillespie's Rule)

Global geometry of the molecule AX_mE_n	Number of binding doublets (m)	Number of non-bonded doublets (n)	Total number of doublets ($m+n$)	Hybridization types	Specific geometry to the molecule	Example
AX_2	2	0	2	Sp		Linear CO_2 – C_2H_2
AX_3	3	0	3	Sp^2		Triangular C_2H_4 , BCl_3
AX_2E	2	1	3	Sp^2		Bent SO_2 , $SnCl_2$
AX_4	4	0	4	Sp^3		Tetrahedral CH_4 , $SiCl_4$, NH_4^+
AX_3E	3	1	4	Sp^3		Pyramidal NH_3 , NF_3 , PF_3
AX_2E_2	2	2	4	Sp^3		Bent H_2O , H_2S

AX₅	5	0	5	Sp ³ d		Trigonal Bipyramidal (TBP) PCl ₅
AX₆	6	0	6	Sp ³ d ²		Octahedral SF ₆