

Covalent Compounds, MOT & VBT

Inorganic Chemistry (2)

5th lecture

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2023-2024

Covalent Compounds

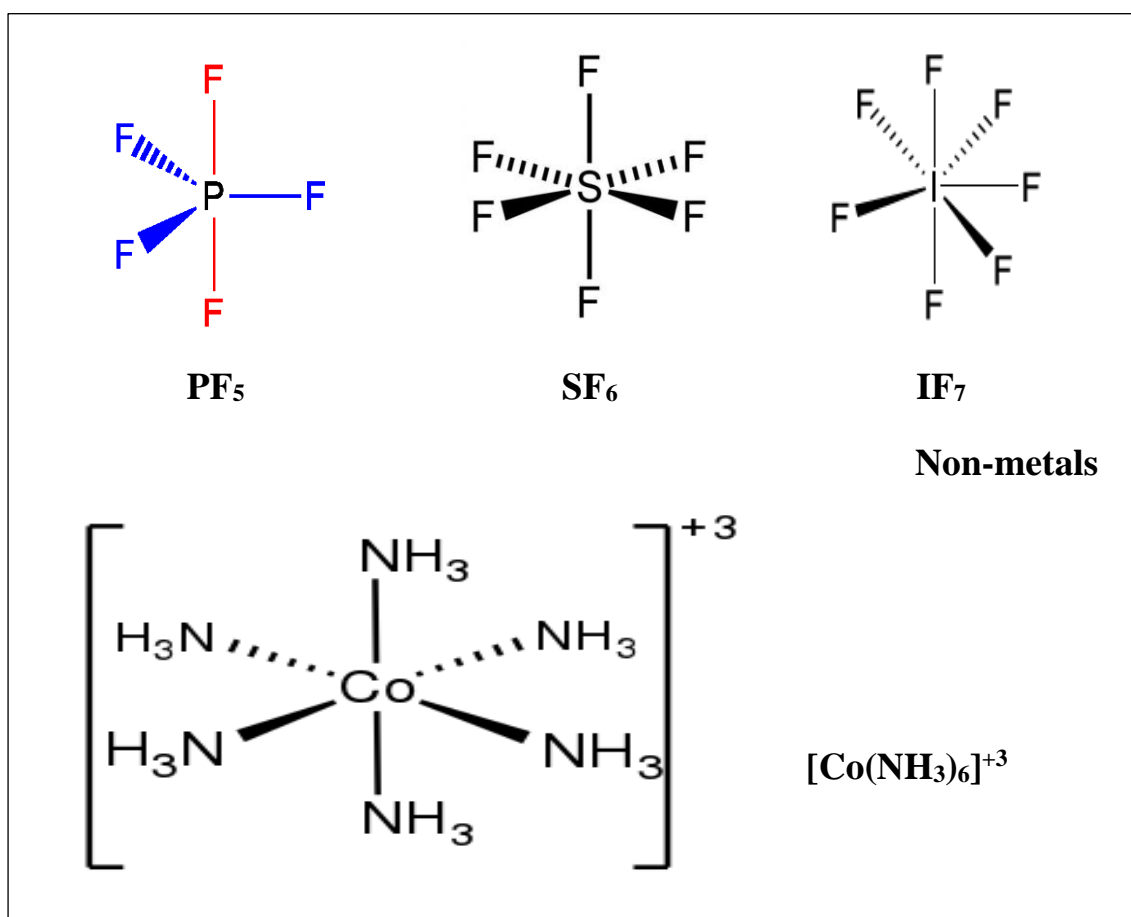
Lewis's definition of a covalent bond is a bond that results from the sharing of two or more atoms with their electrons in an equal or close contribution (the force that connects the two elements is not an electrostatic force), meaning that the electronic cloud does not move from one atom to another.

The modern definition of covalent bond is the amount of changes that occur or occur in energy when two atoms approach each other, so that the energy of the system becomes the least possible when the distance between the two atoms reaches a certain amount. This distance is called the equilibrium distance, and covalent bond can be measured using X-ray diffraction.

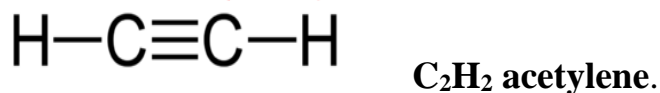
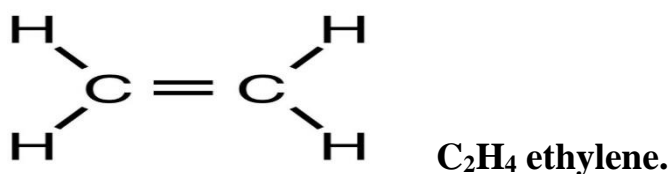
When covalent bond molecules are formed between the **S** and **P** orbital atoms, these molecules have a maximum of electrons equal to eight in their outer shell for each atom, which is called **8** octet rule, making up the molecules, which is called the Lewis octet structure, so the total sum of the outer orbitals = 4 or the sum of total number of electrons in the outer shell = 8, and the total sum of the pairs of electrons involved in the formation of bonds is also 4, provided that the number of electrons in the outer shell of any atom is not less than four electrons, and Lewis theory proves that the formation of a stable compound requires that the atoms reach the noble gas distribution **CF₄**, **NH₃**, **OF₂**, **F₂**. For example, the fluoride method requires two atoms that have reached the required limits for the envelope (that is, each atom has **8** electrons in its outer shell). As for the elements that contain less than four electrons, the octet Lewis structure does not apply to them, as **H** atoms need only two electrons to complete the envelope of the secondary shell from Type **S**. Also, in their covalent compounds, **B** atoms do not reach the noble gas arrangement because they contain three electrons in the shell. Therefore, boron compounds are called incomplete covalent compounds, for example **BF₃**. Therefore, these compounds can interact with a compound in which an element contains a nonbonding ion pair.

The molecule that has the ability to donate an electron double is called a **Lewis base**. The molecule that accepts the donated pair is called a **Lewis acid**. The compounds that contribute to the electron double are called a **Lewis base**. As for the compounds of boron, they are called **Lewis acids**. Lewis proposed calling the bond resulting from boron a coordination bond to fill the electron deficiency in this atom.

For elements that contain a **d-type** secondary shell, their valence shell will move further away from the Lewis octet structure. For this type, the third period scale was established, as many elements have high valence numbers for metals and transition elements, and the number of valence shell electrons is determining covalent bonds can be 5,6,7,8.



Double Bonds of Lewis Structures when more than one pair of electrons is used to form a bond between two atoms, the Lewis molecule can also be completed in an ethylene, acetylene, and nitrogen molecule.



The compound NF_5 does not exist because there is no **2d** shell in the **N** atom, but one of the problems that hindered the application of Lewis rules is the structure of the nitrogen oxide molecule $\text{N}=\text{O}$, **NO**.

Molecular Orbital Theory (MOT)

This theory of the two scientists, Hund and Millikan, differs radically from the valence bond theory, as it assumes that the movement of electrons in molecular systems falls under the influence of a group of nuclei returning to the atoms united to form the molecule.

One of the ways to represent this theory is the linear combination of atomic orbitals (L.C.A.O), which assumes the possibility of combining the atomic orbitals of the united atoms that make up the molecule to give the molecular orbitals. That is, the electrons spend most of the time near one of the two controlled nuclei. If the electron is more likely to return to a particular nucleus, the wave function is described as closer to atomic orbital. As for the wave function for a molecular orbital, it is formed by the linear union of the two wave functions of two separate atomic orbitals, so it is formed by the linear union of two molecular orbitals. That is, the number of molecular orbitals resulting or formed from the union of the two atoms is equal to the number of united atomic orbitals, where two types of molecular orbitals are generated, one of which is of low energy and is called bonding molecular orbitals, it is a result of the sum of the atomic orbitals, which can be represented by the equation:

$$\Psi_b = \Psi_A + \Psi_B$$

Ψ_b = bonding wave function.

Ψ_A = wave function of A atom.

Ψ_B = wave function of B atom.

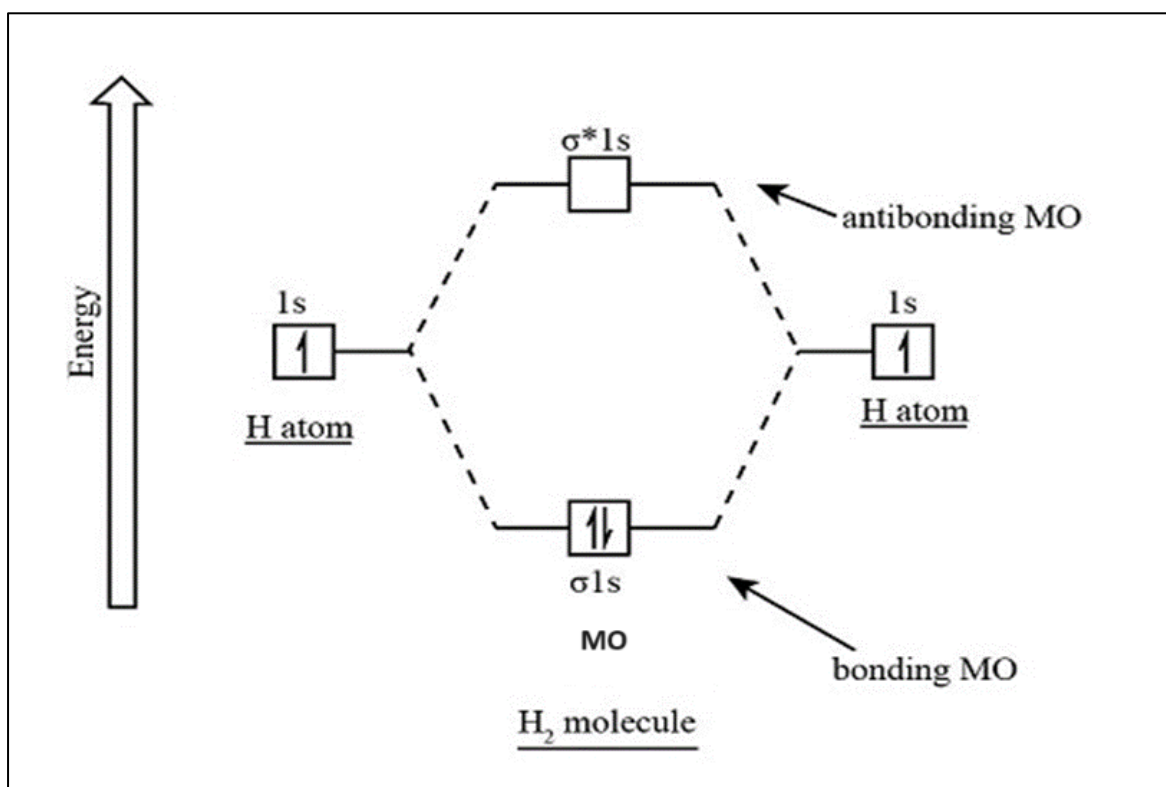
The other molecular orbital with a high energy level is called the antibonding molecular orbital.

$$\Psi_a = \Psi_A - \Psi_B$$

Ψ_a = antibonding wave function.

The molecular orbitals formed are close to the atomic orbitals of the universe b, since the atom possesses atomic orbitals of secondary shells of a type according to the quantum numbers of the atoms or molecules.

The molecule also depends on quantum numbers, and these are called molecular orbitals σ & π .

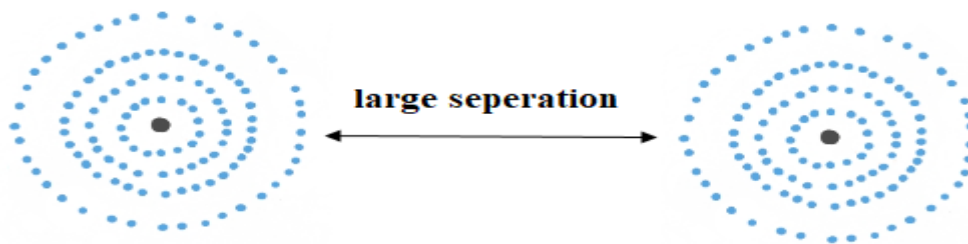


Molecular orbitals are also subject to Pauli's rule of exclusion, and each molecular orbital does not carry more than two electrons. It also follows Hund's rule in distributing electrons, or in other words, the electrons are distributed among the orbitals of equal energy individually, and then the pairing process takes place. If one electron is allowed to be

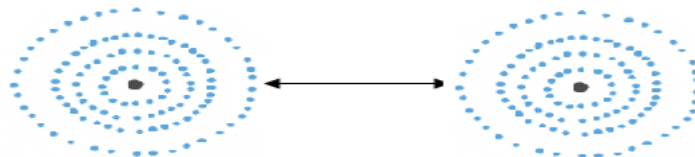
inserted into the bonding and allotropic molecular orbital of a molecule or an ion such as \mathbf{H}_2 , the wave function for the molecule will be as follows:

$$\Psi_{AB} = \Psi_b = \Psi_A + \Psi_B \quad \text{-----(1)}$$

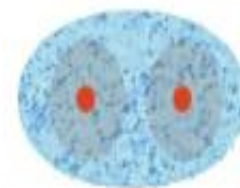
If the \mathbf{H}_2 molecule contains two electrons, it can be represented starting from their presence at a distance so that they are not affected by the electron cloud of either one of the other, but when approaching each other more, the electronic density between the two nuclei will increase as a result of the interference of the atomic orbitals with each other,



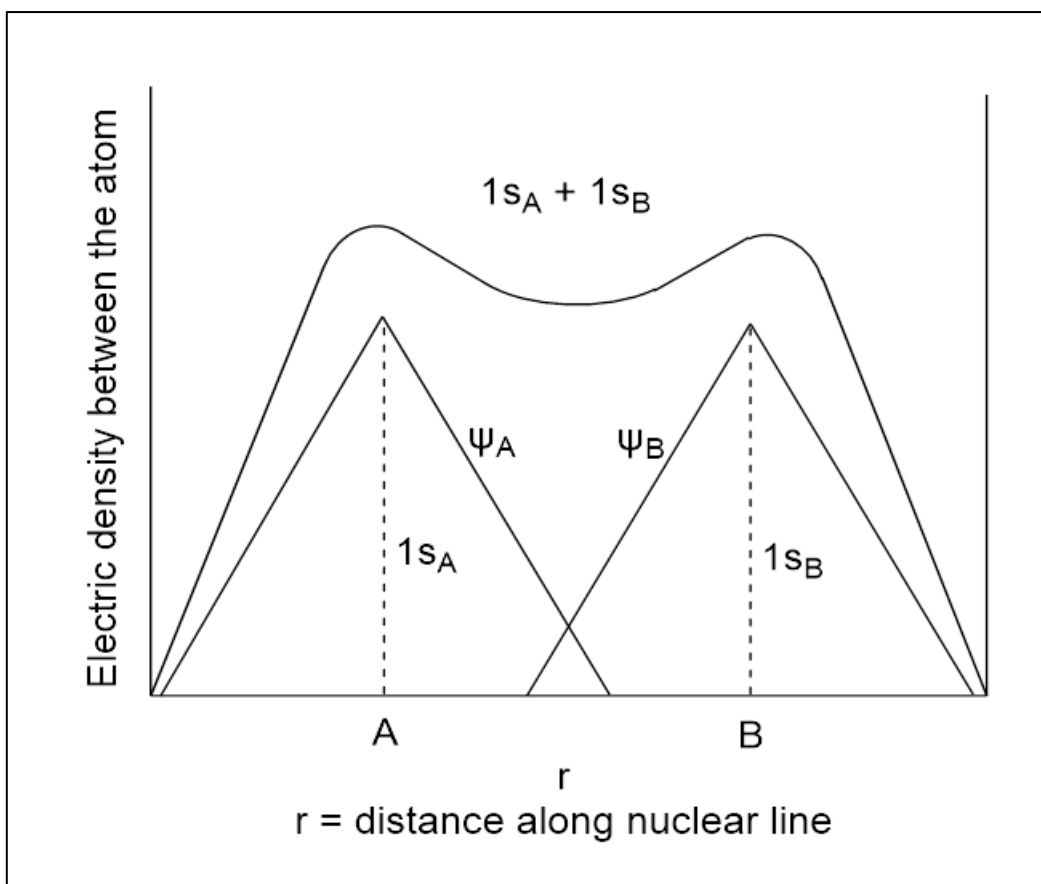
And when the distance between the two atoms decreases further until the state of stability is reached for the two atoms, and the molecular orbital is formed.



The electronic density is distributed to each of the two atoms, and the maximum density of electrons is between the two atoms. The molecular orbital formed is called the bonding molecular orbital.



This orbital is stable, so that it conserves energy for the system, which increases the stability of the molecule. If the molecular orbital formed is a linear combination of the orbital functions of two atoms $\mathbf{H}_{A1}, \mathbf{H}_{B2}$, as in the following diagram:



The total wave function is equal to the product of the two functions for each of the two electrons.

$$\Psi_{\text{Molecular}} = \psi_b^A \times \psi_b^B \quad \text{-----(2)}$$

This means that there is no distinction between the two electrons, which leads to:

$$\Psi_{\text{Molecular}} = (\psi_A^1 \psi_B^1) \cdot (\psi_A^2 \psi_B^2) \quad \text{-----(3)}$$

$$\Psi_{\text{Molecular}} = \psi_A^1 \psi_A^2 + \psi_A^1 \psi_B^2 + \psi_B^1 \psi_A^2 + \psi_B^1 \psi_B^2 \quad \text{-----(4)}$$

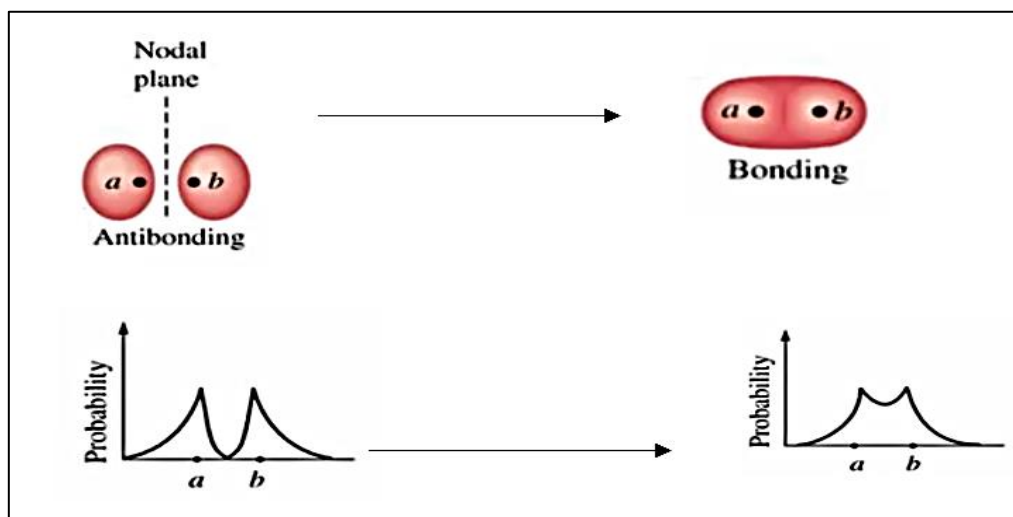
ionic cov. cov. ionic

It is noted from the last equation that there are two terms, one of which is covalent, represented by the two structures $\psi_A^1 \psi_B^2 \psi_B^1 \psi_A^2$, and the other is ionic, represented by the two structures $\psi_A^1 \psi_A^2 \psi_B^1 \psi_B^2$. This confirms the similarity the results of the first theoretical (V.B.T) and the second theoretical (M.O.T).

However, it is noted that molecular orbital theory confirm the ionic terms in such a way that it is not equal to the covalent terms because it did not take into account the repulsion that occurs with the electrons. Therefore, the theoretical values of the bond energy and the distance between the two atoms are not consistent or identical with the practical values except after making corrections to equation 4, and these corrections are shown in the following table.

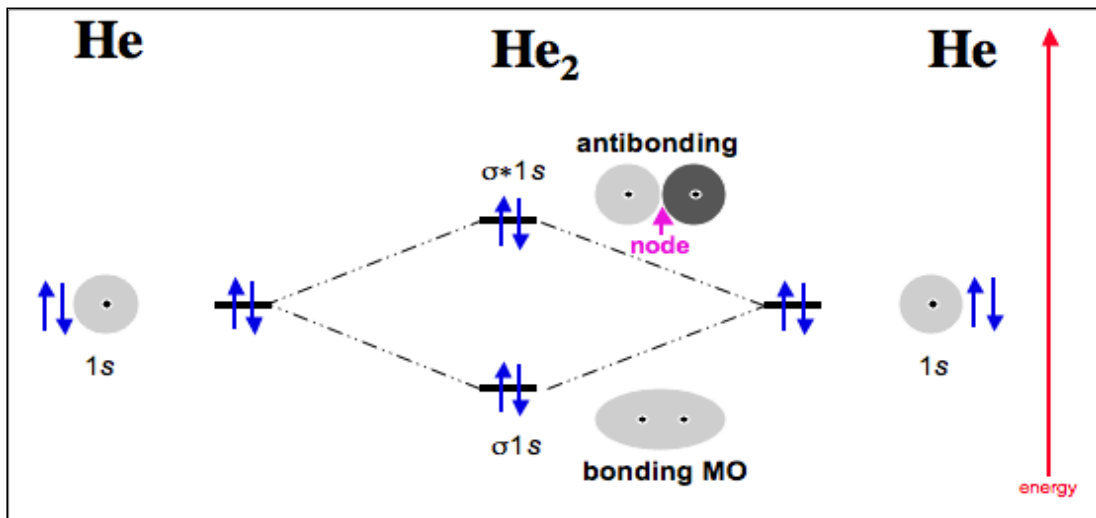
Bond length Å°		Bond energy eV	Wave function
0.85	Theoretical value	2.70	$\Psi_b = \psi_A + \psi_B$
0.73		3.49	
0.741	Experimental value	4.11	+* Shielding electron effect
0.741		4.747	

Explaining the hydrogen molecule to the allotropy orbital shows that the electrons spend most of their time in the overlap region between the two atoms H_A & H_B , which makes the attraction between the two electrons and the two nuclei as great as possible, so that the energy level of ψ_b is lower than the energy level of the atomic orbital.

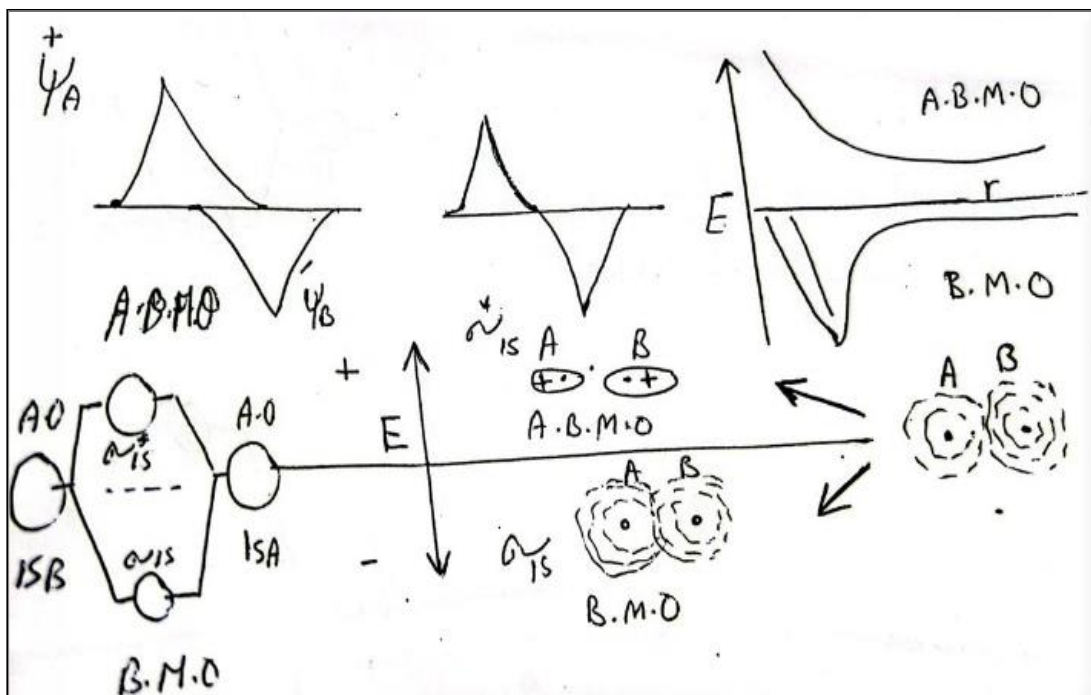


However, if we assume that the molecular orbitals between the two atoms contain more than two electrons, such as the two atoms of helium and He_2 , then two of the electrons occupy the molecular orbital **B.O.M**, giving a molecular orbital of the sigma type σ^b , while the other two

electrons occupy the molecular orbital with the anti-bonding type σ^* , and it was later shortened to σ^* which high-energy one shortened σ to σ^b .



Where the electronic density decreases in the overlap region, as the electrons are pushed further from the area between the two nuclei, and the electronic density is as **low** as possible (so that it reaches zero) in a level called the **nodal level**, which is perpendicular to the line connecting them. As a result, the repulsion between the nuclei of the two atoms increases, and the molecule is made. The first is stable, meaning that the anti-corrosive molecular orbital is less stable and has a higher energy than the atomic orbitals that make it up.



When representing the energy levels between two atoms according to the molecular orbital theory, equivalent orbitals are placed together, taking into account that the most stable levels are in the lower position. If the two atoms are of the same element, then molecules such as He_2 , He_2^+ , H_2^+ , H_2 are formed by linear combination. If the electrons are located in the molecular orbitals of the two atoms, this means that they spend most of their time between the nuclei of the two atoms. However, if they are located in the molecular orbitals of the opposite nature, then they spend most of their time away from the nuclei. In this way, the bond order and the magnetic character of the molecule can be known.

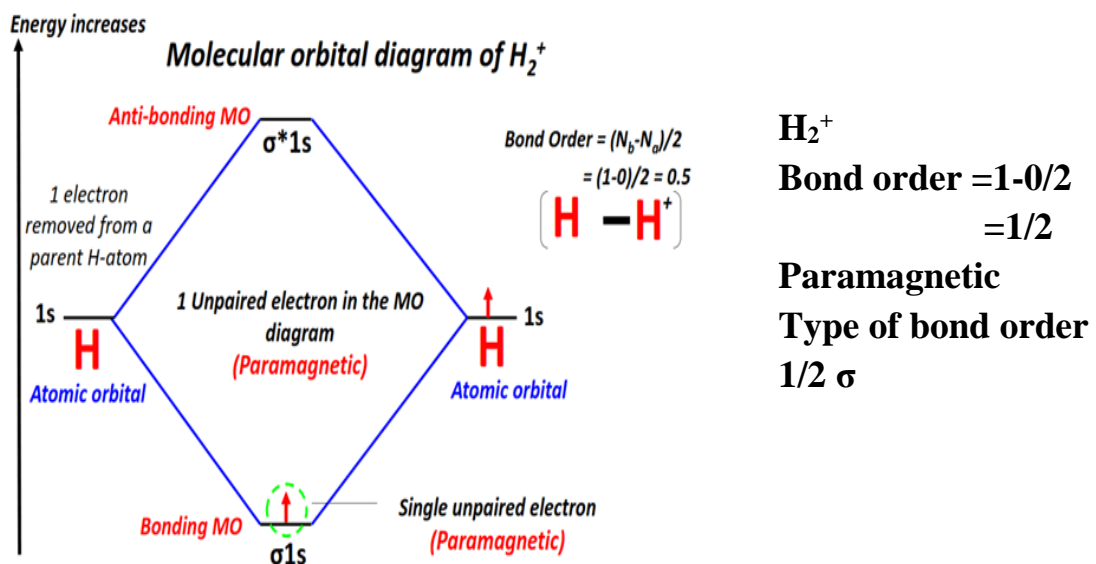
رتبة
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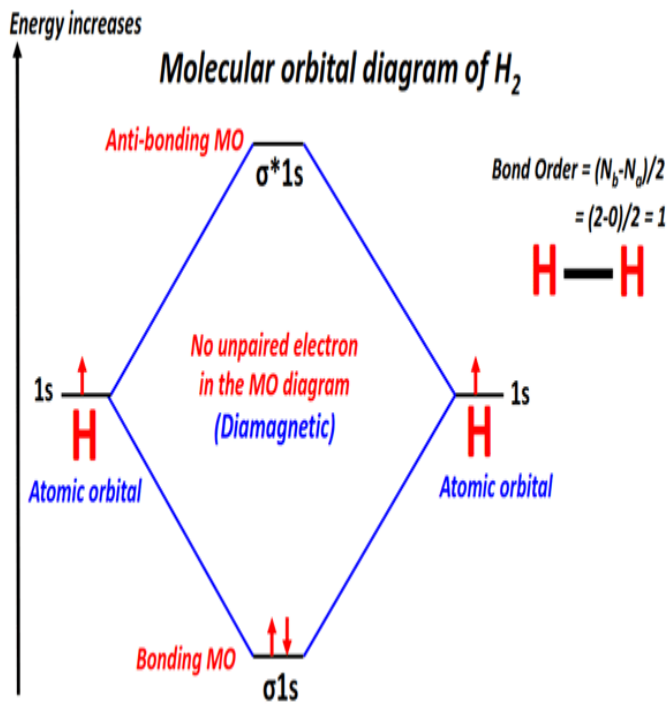
$$[\text{Bond order} = \frac{\text{No. of electrons in B.M.O} - \text{No. of electrons in A.B.M.O}}{2}]$$

قانون
حفظ

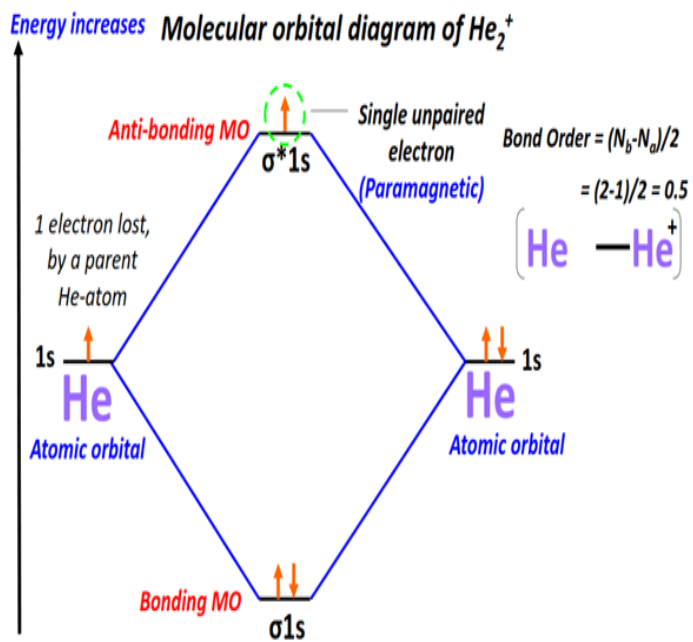
The first bond that is formed is of the sigma σ type, and the bonds that are formed after it are of the π type. If the bond order is equal to $1/2$, it is also of the sigma type. If the bond order is = 2 , then it is of the sigma σ type, but when it is equal to $1 \frac{1}{2}$, it means the presence of one bond sigma σ type and half of bond π type.

H_2^+ , H_2 , He_2^+ , He_2

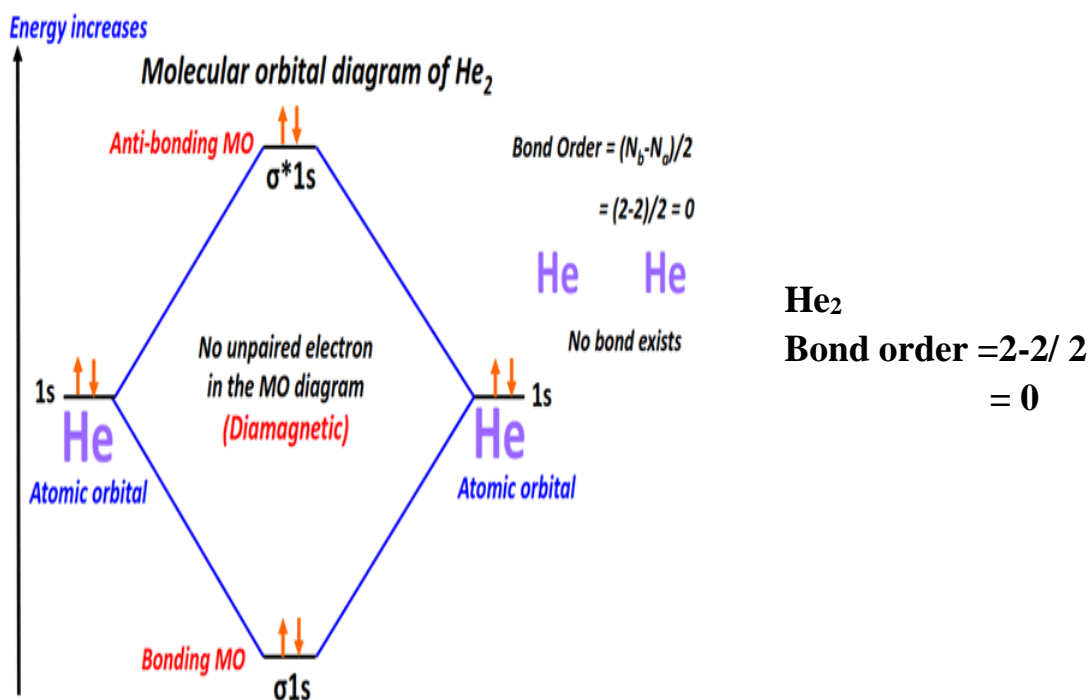




H_2
Bond order = 1
Diamagnetic



He_2^+
Bond order = $2 - 1/2$
 $= 1/2$
Paramagnetic



If the molecule contains single electrons, it has paramagnetic properties, but if it contains double electrons, it is repulsed by the magnetic field and is called diamagnetic. Therefore, both of He^{+2} , H_2^+ are paramagnetic, while H_2 the magnetic characteristic has no relation to the stability of the molecule.

The two most important conditions that must be met in the formation of a molecule from the linear interference of atomic orbitals are:

1. The interference between atomic orbitals must be a wave.
2. For effective interference to occur between the orbitals of different atoms, the orbital energies of the two atoms must be approximately equal.

Regarding the first condition, the interference is considered very important, although it is not sufficient to form the bond. The interference is symbolized by the letter **S** and expressed mathematically as follows:

$$S = \int \psi_A \psi_B dT.$$

It is a measure of the extent to which the wave function of one of the two atoms overlaps with the wave function of the second atom, and then

the distance between the two atoms is infinity, which is a non-bonding case.

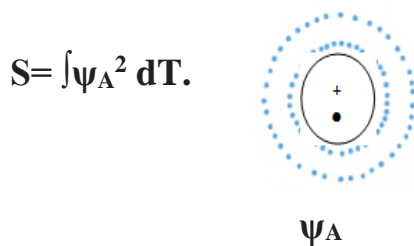
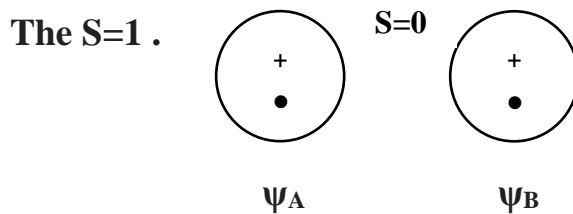
When $S=0$ non-bonding.

When $S < 0$ Bonding.

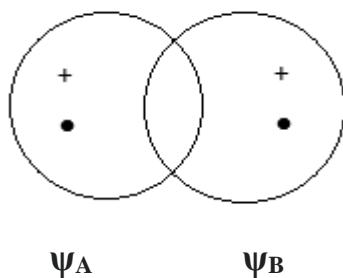
When $S > 0$ Antibonding.

$S =$ value of linear overlapping orbital

When the distance between two nucleus= 0



In this case, both ψ_A and ψ_B correspond to the same wave for one of the two atoms. However, when the distance between the two nuclei is an intermediate between the two values, that is, between zero and infinity, the value of S is positive and an intermediate between **zero** and the integer **1**, we obtain a state of bonding due to the positioning of the two electrons between the two nuclei.



In the case of antibonding, it causes the two electrons to repel and move away from each other and from the nuclei of the two atoms, so the value of S is less than **zero**.

It is known **that the best way to estimate the strength of the bond is by measuring the energy released when the bond is formed**, which is difficult most of the time, but the scientist Pauling invented a method **that depends on the interference between the orbitals of the two atoms that make up the bond**, whether this interference is positive, negative, or equal to zero, along with knowing **the amount of this interference. Between atomic orbitals and this interference depends on:**

- 1- Energy of overlapping orbital.
- 2- Size of overlapping orbital.
- 3- Distance between two nucleuses.
- 4- Symmetry of overlapping orbital.

The values of ℓ are used to obtain the following:

- 1- Calculating the orbital angular momentum, which is a vector and constant value within one secondary plane.

$$n\ell = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi}$$

This does not mean that the electron is at rest when the momentum = 0, but the resultant angular momentum = 0 because the momentum is the value of its vector and represents the angular momentum $\mu\ell$ resulting from the movement of the electron around the nucleus in the secondary level ℓ .

$$\text{When: } \ell=1 \rightarrow \mu\ell = \sqrt{\ell(\ell + 1)} \frac{h}{2\pi} = \sqrt{\frac{2h}{2\pi}}$$

$$\text{When: } \ell=2 \rightarrow \mu\ell = \sqrt{2(2 + 1)} \frac{h}{2\pi} = \sqrt{\frac{6h}{2\pi}}$$

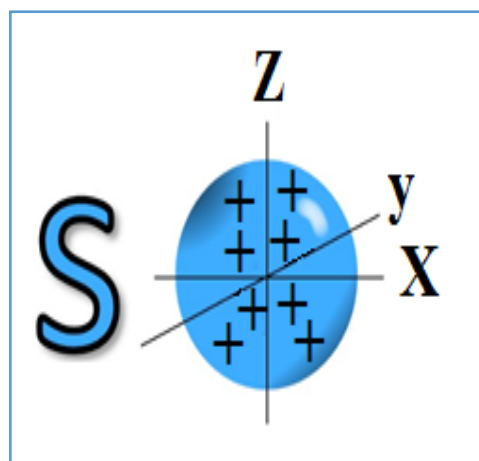
- 2- **Determine the shape of the secondary orbitals.**

The shape of the secondary orbital is determined by knowing the probability of the electron being present through the wave function determined by the angular function and the diagonal function, that is, depending on r, Θ, ϕ with x, y, z , which is represented by the number of electrons from the center of the atom and the angles it forms with the axes. This is done by determining for the knots formed by the electron movement and extracted from the following equation:

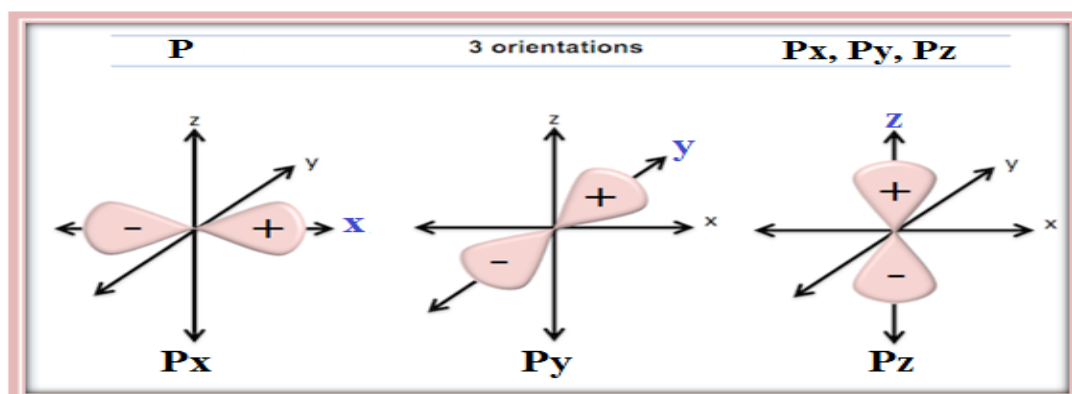
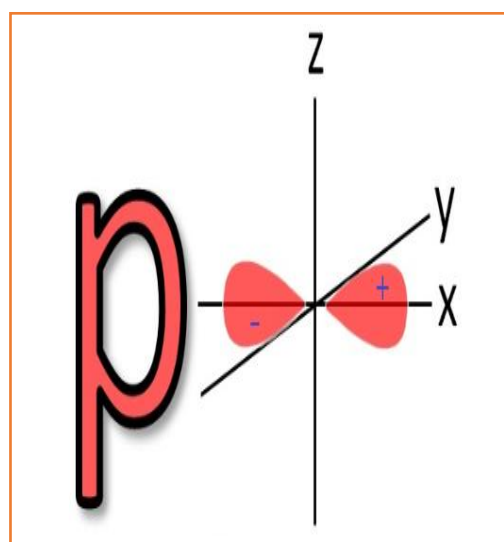
no. of lobes = ℓ

It exists within the three axes: x, y, z.

If $\ell = 0$, then the number of nodes = 0 and the orbital is of the S type and its shape is spherical or circular, meaning that it has a diagonal function only, and since the resultant of its angular momentum = zero, it is regular symmetric within the three dimensions or axes, and regular symmetry is given the symbol (g) (gerada) and when $\ell = 1$, then the number of nodes = 1.

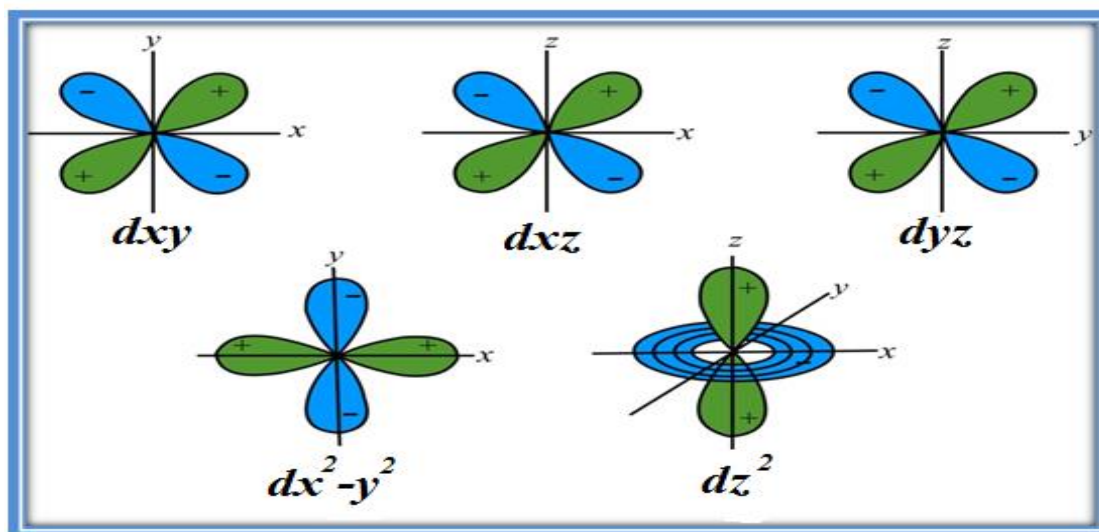


The orbitals of the secondary level are of the p type, and their number is three orbitals called Pz, Py, Px, each of which has a node, meaning that the probability of the presence of the electronic density is in the following form, that is, the sign of the wave function changes, and the symmetry is non-spherical, and the probability of the presence of the electronic density and its distribution changes with the change of the angular function and the function. The diagonal is within the Cartesian axes x, y, z for each orbit, and the three (p) orbitals are distributed perpendicular to the three axes:



Orbitals (p) do not have spherical symmetry, but consist of orthogonal lobes of asymmetric sign in the wave function and are symbolized by (u) (ungerada), i.e. the wave function sign changes for each orbital of the p orbitals.

When $\ell = 2$, then the number of orbitals of the secondary level (d), and it has five orbitals, each containing two nodes, that is, for each orbital of the d orbitals, it contains two orthogonal nodes. Opposite to each other, they are symmetrical, that is, the symmetry becomes of the type g, and it is as in the p orbitals, the wave function changes with $m\ell$, ℓ , r, and the shape of the four d orbitals is identical or similar.



As for the fifth orbital, d_{z^2} , it is located on the z axis. The electronic density, or the presence of the wave function, is as large as possible on the z axis above and below the axis, and the electronic density is less on the Wave $d_{z^2-x^2}$, $d_{z^2-y^2}$. When $\ell = 3$, the number of nodes = 3, meaning that the wave function is unified by the values of ϕ , Θ , r, and the wave function has irregular symmetry (ungerada). Every principal quantum number (n) contains a number of orbitals, which can be known from the following equation:

$$\text{no. of orbital} = n^2, \text{ When } n=1$$

All values of the secondary quantum number ℓ for any primary quantum number n are equal in energy before the magnetic field is applied or if they are empty.

- 3- The secondary quantum number ℓ determines the energy of the electron in the secondary energy level.

$$\text{When } \ell = 0, 1, 2, 3, 4$$

$$s < p < d < f$$

- 4- Each secondary energy level contains a maximum number of electrons depending on the principal quantum number. no. of electron = $2n^2$.

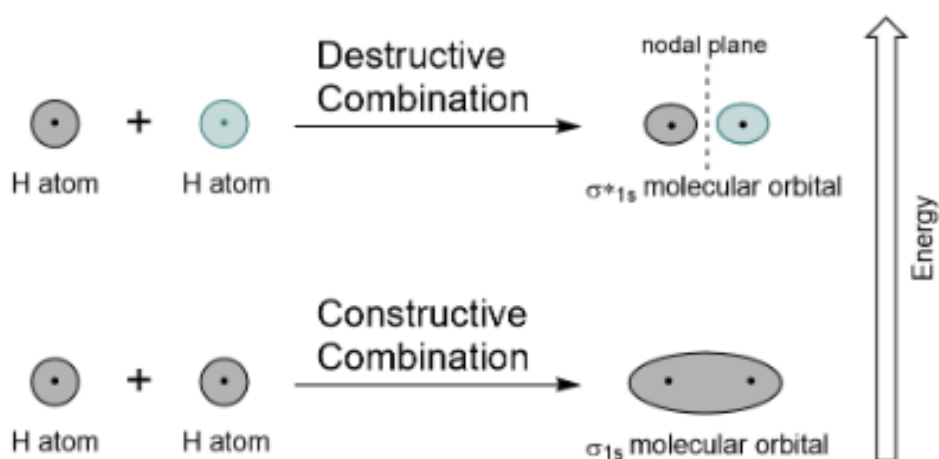
Since each secondary level contains a number of orbitals, which = $2L + 1$, these electrons for each secondary level are distributed among the orbitals so that each orbital does not take more than two electrons.

- 5- Since each principal quantum number n contains a number of secondary levels, the determination of the energy of any electron is based on the principal quantum number n formed by the secondary. Based on the rule that the lowest-energy secondary shell is filled first.

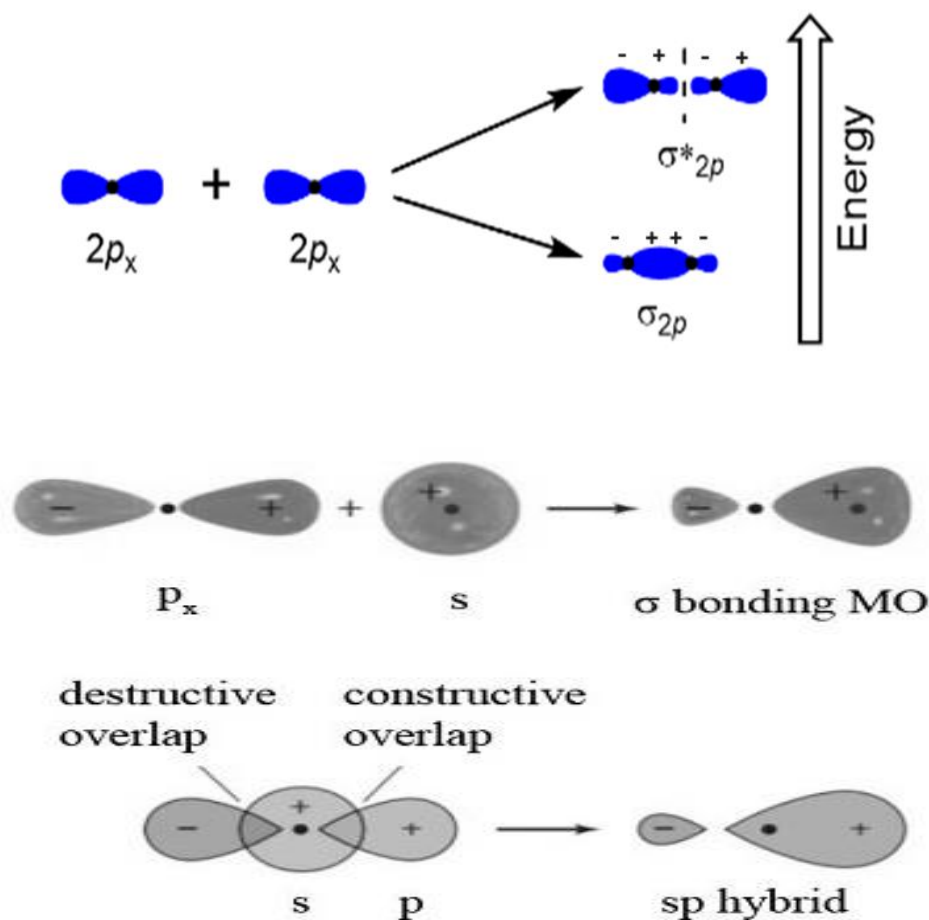
Symmetry of Molecular Orbital and Types of Linear Combination and Overlapping

Symmetry of molecular orbitals and types of linear interference:

Sigma σ orbital is a molecular orbital with cylindrical symmetry around the molecular axis between the two nuclei. If the nuclei are two similar atoms of the type **S** and **P** orbitals, then the molecular orbital is formed between the two atoms.

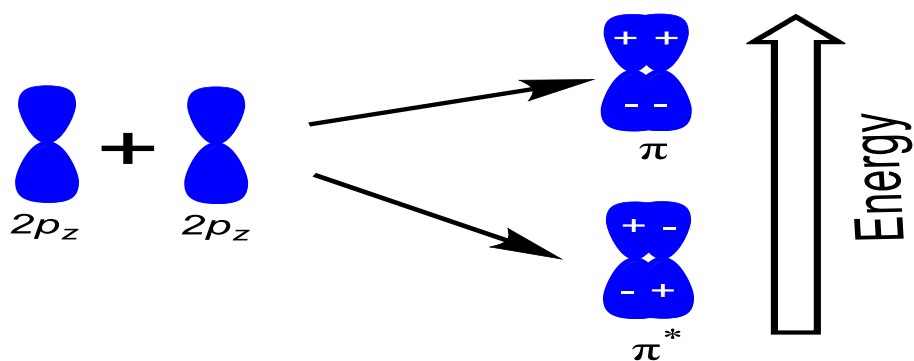


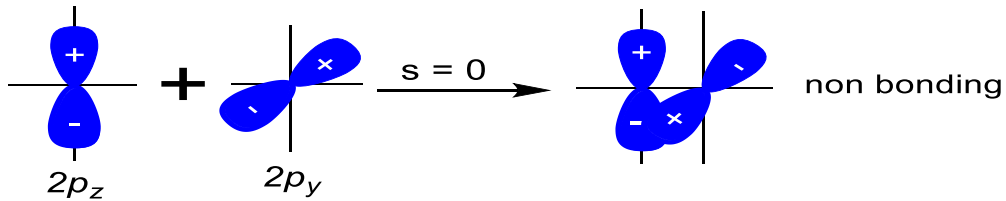
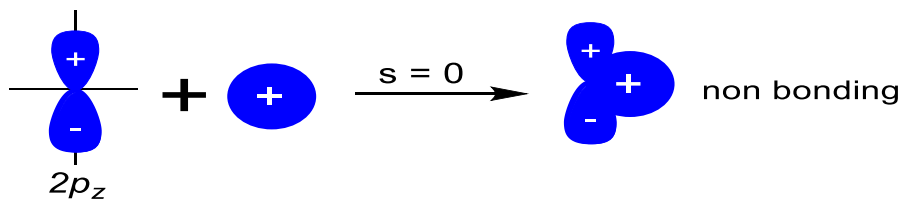
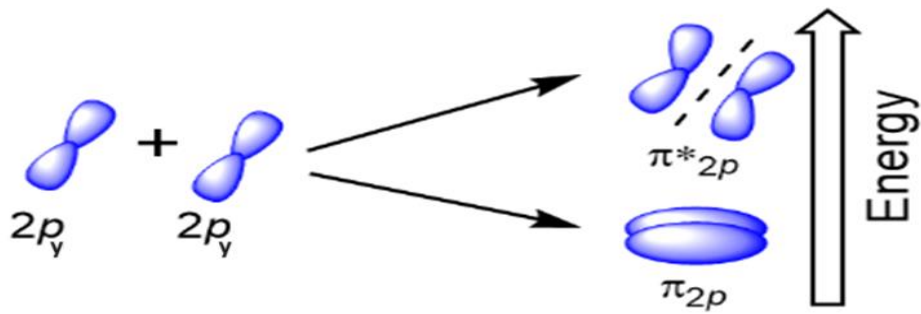
The sigma molecular orbitals also consist of the linear union between the **P_x** orbitals, specifically the **P_x** type, arranged along the x axis between the two nuclei, so they have the same sign. The electronic density is highest possible in the bonding region, but against bonding, the electronic density is reduced and the energy level becomes higher than that of atomic orbitals.



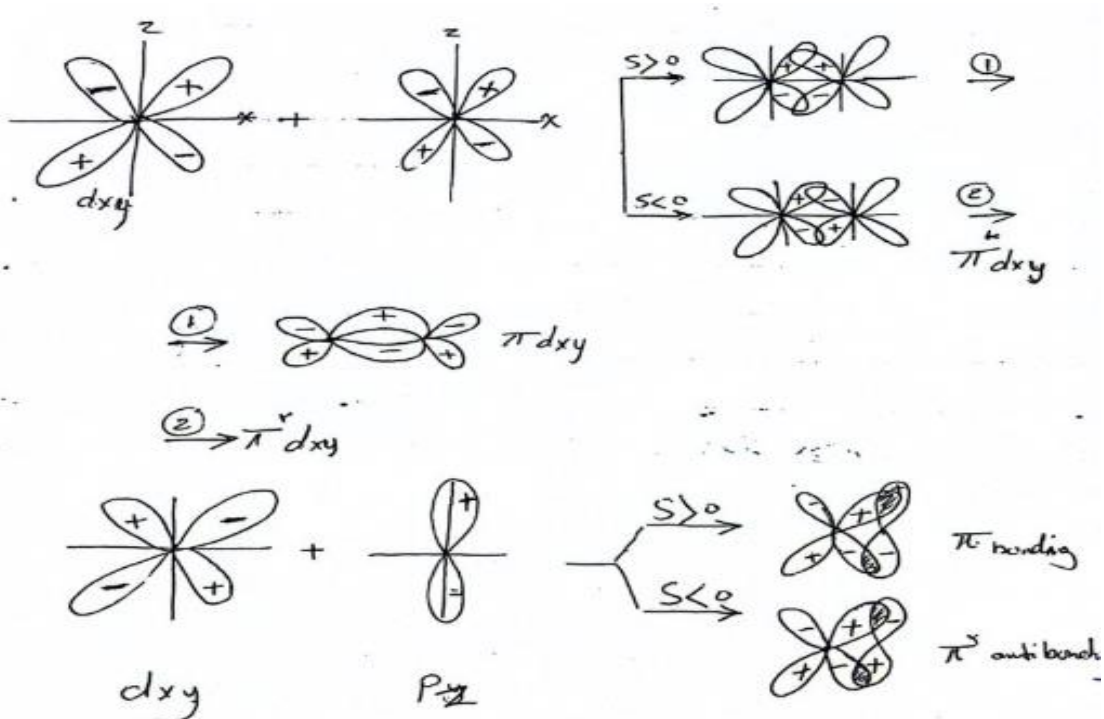
π orbital

In atoms containing **p** orbitals, the union of **Py** with **Py** orbitals, or **Pz** with **Pz** orbitals, that are parallel to each other, leads to interference from the top and bottom of the line connecting the nuclei of the two atoms and the level of the bond (the level of the knot formed by the type of π). The electronic density in the π orbitals is distributed on two opposite sides in a sign and the wave symbol.





The molecular orbital is of the πp type (bonding) of the irregular symmetry type (ungarada), similar to a flip around the center of the molecule, while the π^* type is of the regular type d-type orbitals consist of the following form:

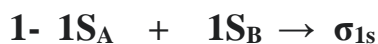


Lateral overlap occurs between two parallel orbitals and the type of bond formed is (π).

$$\left. \begin{array}{l} dx^2-y^2 + dxz = \\ + dyz = \\ + dz^2 = \end{array} \right\} S=0 \text{ nonbonding.}$$

$$\left. \begin{array}{l} dxy + S \\ dyz + S \end{array} \right\} S=0 \text{ nonbonding}$$

or the sequence of energy levels of similar atom molecules containing **S** and **P** type orbitals.

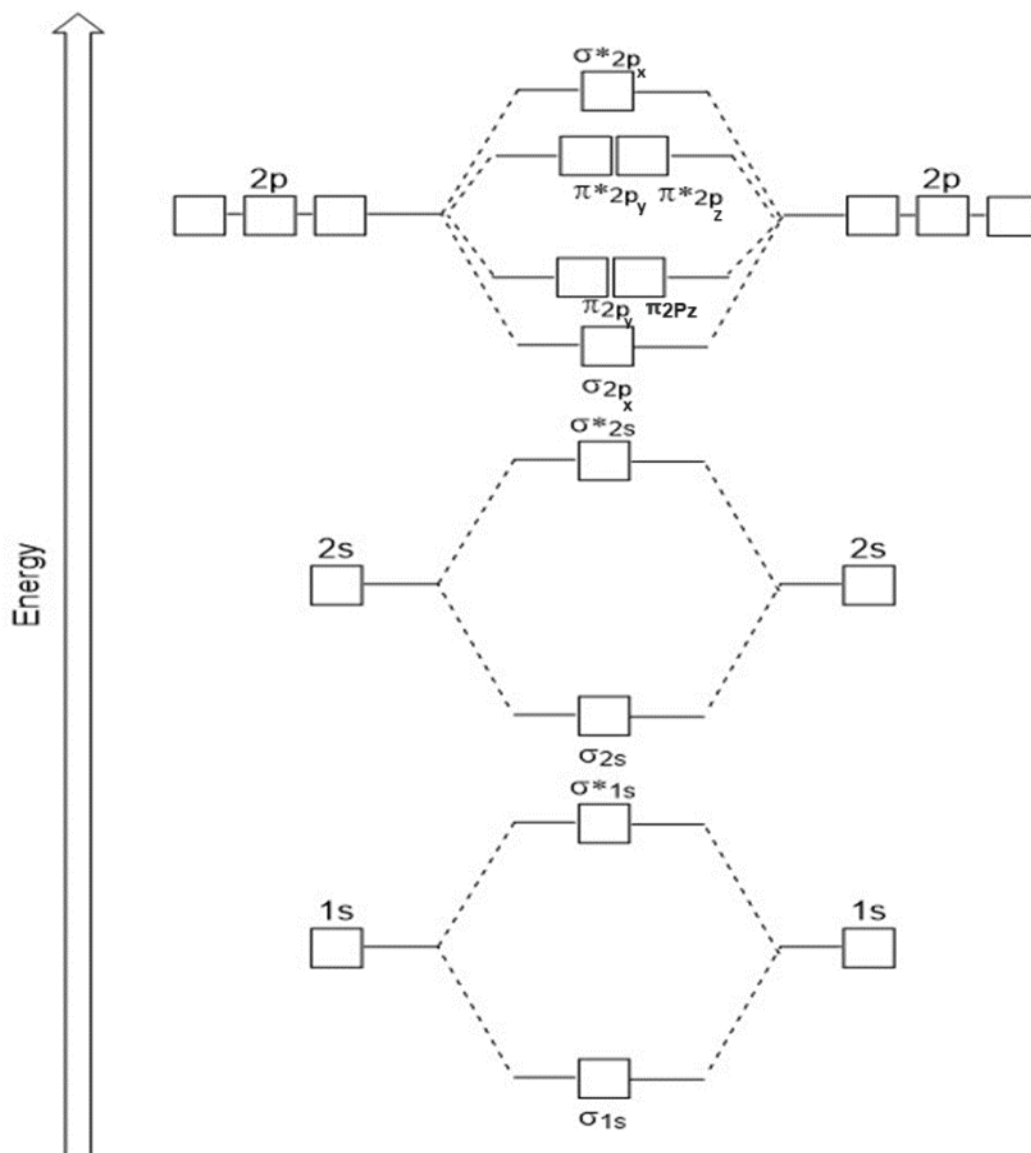
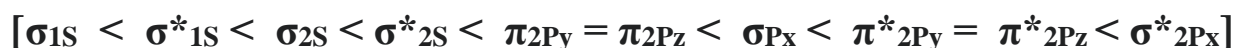


Energy difference

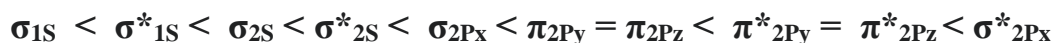
**Their energies are equal,
so when filling these two
orbitals we must observe
Hund's rule**

Both π_{2Py} & π_{2Pz} exist at the same energy level, as is the case for π^*_{2Pz} & π^*_{2Py} . Therefore, when filling electrons, Hund's rule must be observed. If the atoms are small, the energy level π_{2Pz} & π_{2Py} will be lower than the energy level σ_{2Px} because in small atoms there is a convergence between the **2S** & **2P** energy levels, and the opposite happens in large atoms.

Therefore, the distribution of electrons among the molecular orbitals in boron and carbon is as follows:



While for N, O and above, the distribution of molecular orbitals is as follows:

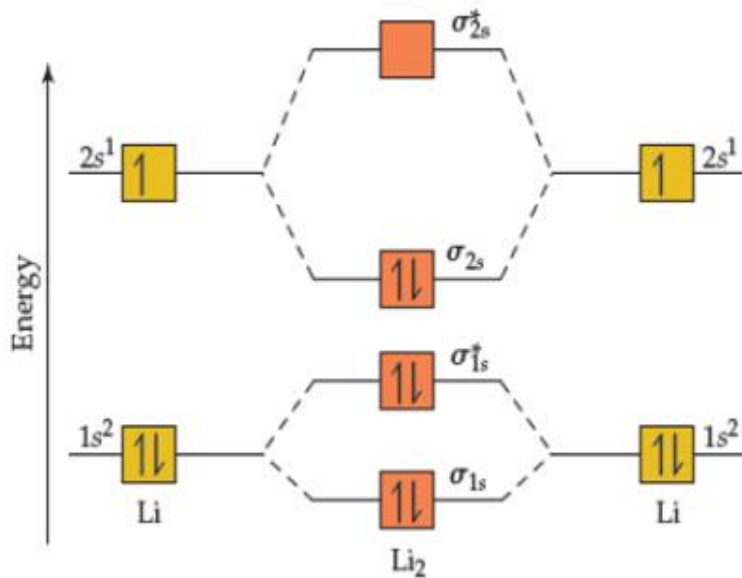


Energy sequence \longrightarrow

المخطط للحفظ

Example: Do these molecules exist, do these molecules have magnetic properties, and what is their stability if they are present? Li_2 , N_2 , O_2 .

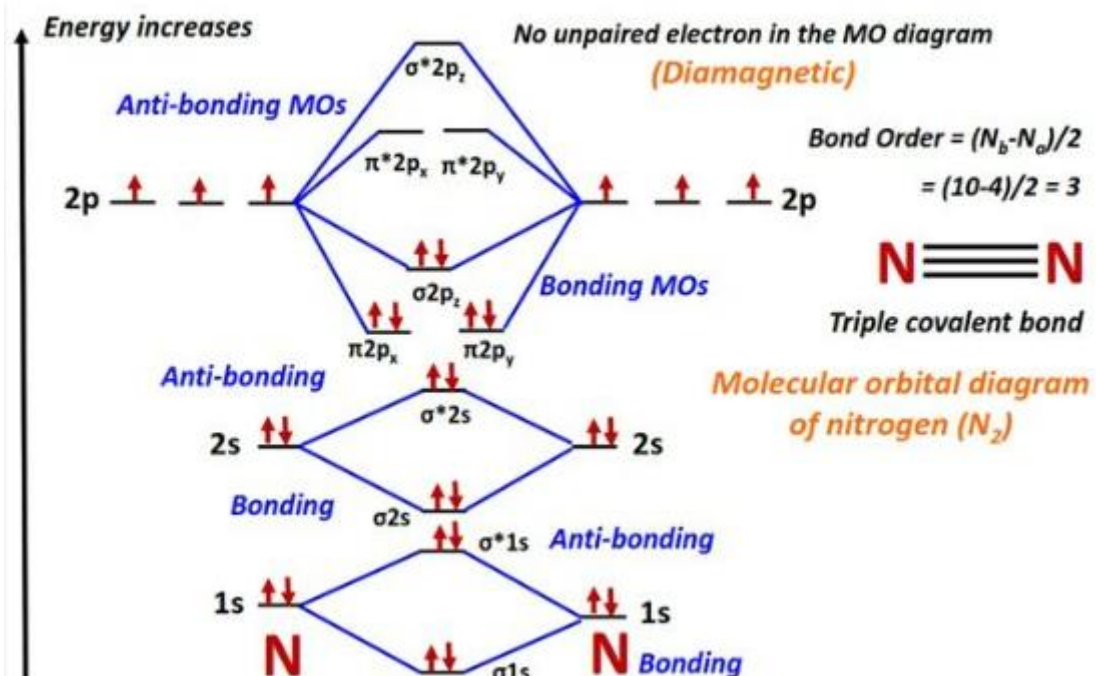
$3\text{Li}: 1s^2 2s^2$

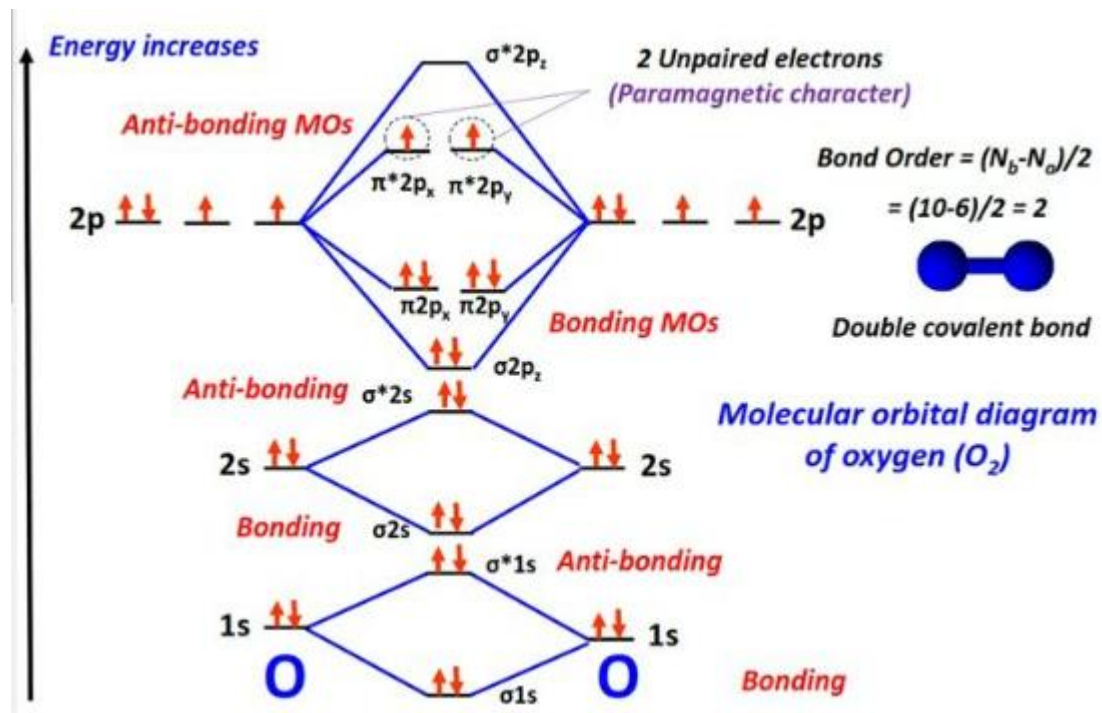


Li_2

$$\text{Bond order} = \frac{4 - 2}{2} = 1$$

The magnetic character depends on the number of individual electrons. Since the molecule does not contain individual electrons, this molecule has diamagnetic properties.





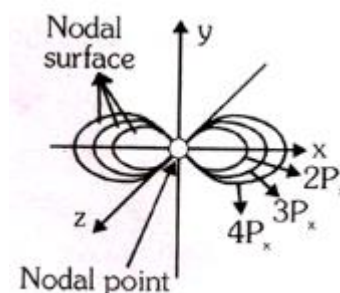
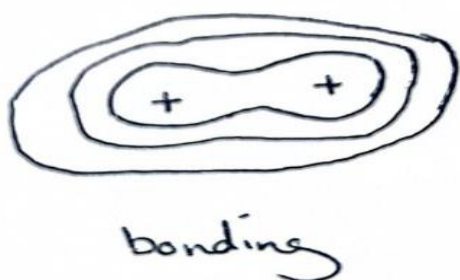
Assignment: Are the following molecules exist or not exist? Then calculate the rank of the bond Ne_2 , F_2 and the magnetic characteristic?

Overlap:

$$\Psi_b = \psi_A + \psi_B \quad \psi: \text{wave function}$$

$$\Psi_a = \psi_A - \psi_B$$

The integral $\int \psi_a \psi_b dt$ is known as the overlap integral S , and is very important in bonding theory. In the bonding orbitals the overlap is positive and the electron density between the nuclei is increased, whereas in the antibonding orbital the electron density between the nuclei is decreased. In the former case, the nuclei are shifted from each other and the attraction of both nuclei for the electrons is enhanced. This results in a lowering of energy of the molecule and is therefore a bonding situation, in the second case, the nuclei are partially barred toward each other and the electrons tend to be in those regions of space in which mutual attraction by both nuclei is severely reduced.



$S > 0$ - bonding

$S < 0$ - antibonding

$S = 0$ - non bonding

The strength of bond will be roughly proportional to the extent of the overlap of the atomic orbitals. This is known as the overlap criterion of bond strength and indicated that bonds will form in such a way as to maximize overlap.

In **S** orbital the sign of the wave function is very were the same (with the exception of small intranodal region for $n > 1$) and so there is no problem with matching the sign of the wave functions to achieve positive ways of arranging the orbitals, some resulting in positive overlap some in negative overlap and some in which the overlap is exactly **Zero**. Bonding can take place only when the overlap is positive.

Bond order: The bond order is defined in MO theory as the number of electron pairs occupying bonding MO's Minus number of electron pairs occupying antibonding MO's, thus the bond orders in H_2^+ , H_2 , HHe , He_2 , $1/2$, 1 , $1/2$, 0 respectively.

The hydrogen molecule is considered more stable than the lithium molecule Li_2 . Likewise the boron B_2 molecule is considered more stable than the Li_2 molecule for the following reasons:

1. The bond of the hydrogen molecule is shorter and stronger than the bond of Li because the radius of the Li atom is larger than the radius of the H atom because the Li atom is located in the second period. Also, the molecular orbital of the H_2 molecule σ_{1s} is closer to the nuclei of the two H_2 atoms relative to the molecular orbital σ_{2s} of

the **Li** atom, where it is the nuclei of the **Li** atom are two groups larger than the nuclei of the **H₂** atom, so their attraction to the orbital is less than that of the **H₂** molecule.

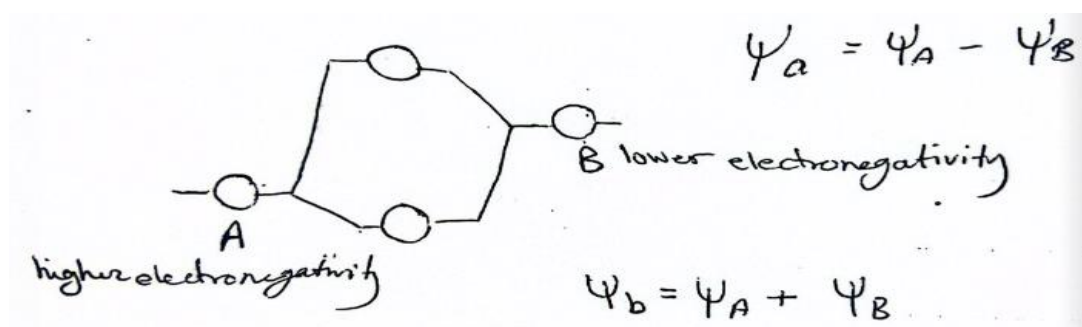
2. The bond energy is higher in the boron molecule than in the lithium molecule, and the bond length in the boron molecule is shorter than the bond length in the lithium molecule because the radius of the boron atom is smaller than the radius of the lithium atom, and this results from an increase in the effective charge **Z*** of the boron atom.
3. The length of the bond increases and its energy decreases with the increase in the atomic number within one group, and the length of the bond shortens and its energy increases with the increase in the atomic number within one period.
4. All alkali metal molecules, from **Li₂** to **Cs₂**, have a bond rank equal to one, and their magnetic properties are of the diamagnetic type, and the same is true for the halogen elements.

General Notes: ملاحظة هذه المعلومات

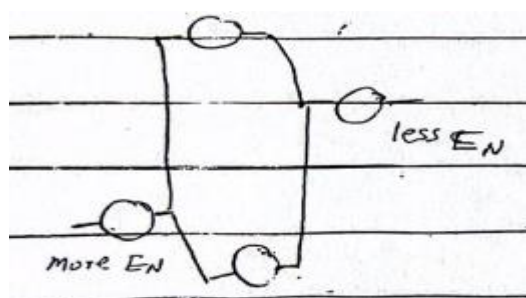
1. When calculating the bond order, the electrons in the (non-bonding orbital) are not included in the calculation, and the energy level of these orbitals is the same as the energy level of their possible atomic orbitals. This results from the fact that these orbitals are not similar in orbital symmetry, so the process does not contribute in bonding process.
2. Heterogeneous molecules that are diatomic of the type (**np, ns**). The bond formed between the atoms of the two different elements means that they are different in their electronegativity values, as well as that they are different in the effective charge, even if the two elements belong to the same cycle, such as **N, O**. This leads to a change in the energy level of one of them is relative to the energy level of the other element. For an element with high electronegativity, the orbital energy level is lower than the atomic orbital energy level for an element with low electronegativity.
3. The contribution of the more electronegative element to the formation of the allosteric molecular orbital is greater than the contribution of the less electronegative element. This means that the energy level of

the allotropic molecular orbital is closer to the energy level of the other, more electronegative element $F \bullet - \bullet H$.

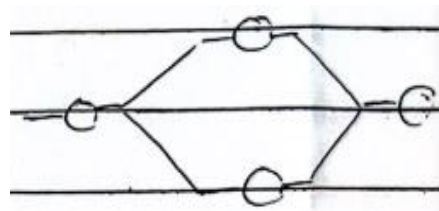
- The contribution of the less electronegative element to the formation of the anti-electronic molecular orbitals is greater than the contribution of the more electronegative element. This means that the energy level of the anti-electronic molecular orbitals is close to the energy level of the less electronegative element, and therefore the electrons of the anti-electronic molecular orbitals spend most of their time near the less electronegative element.



- Non-bonding electrons appear if the two elements are from different spins and maintain the same level.
- As the difference in electronegativity increases, the covalent character decreases, the polarity of the bond increases, and the ionic character gradually appears. For example, CsF and $CsCl$ ionic compounds, that is the energy of the mutual influence of exchange energy, the nuclei of the two atoms on the covalent electrons decreases as a result of the difference in energy levels.



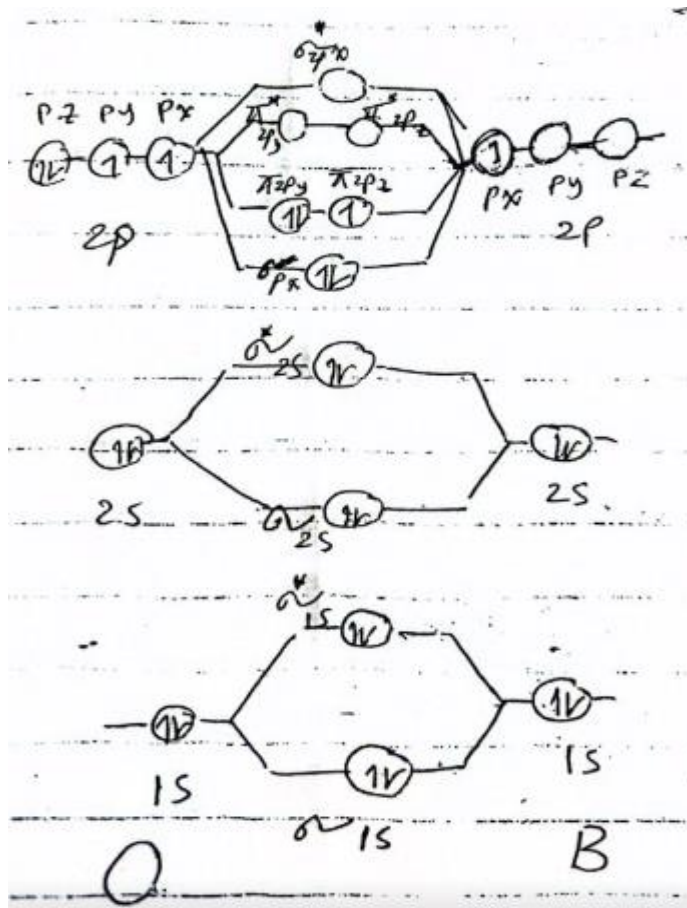
Increased ionic character and decreased covalent character.



100% It has covalent properties because there is no difference in electronegativity. 100% covalent bond.

The arrangement and characteristics of the energy levels in molecules consisting of two different atoms within the same period **ns np**:

- 1. The energy and the bond order increase and its length shortens as the number of bonding molecular orbitals increases at the expense of anti-bonding molecular orbitals.**
2. The bond energy increases as the radii of the atoms that make up the molecule decrease, and its length decreases as well.
3. If the bond order = $1/2$ or 1, it is a bond type, and if it is equal to more than one it means it is a bond type σ + part of the type π .
4. If two molecules are equal in bond order, so the preference for one over the other in terms of stability is based on the following:
 - i- Total nuclear charge (positive is more stable than neutral and neutral is more stable than negative) because increasing the density of the positive charge of the molecule leads to an increase in the attraction of the nuclei of the two atoms to the electronic clouds they share the negative charge on the molecule leads to increased blocking on the two nuclei, and as a result of the repulsion with the other electrons, the length of the distance between the two atoms increases, so the stability of the molecule decreases and the bond lengthens.
 - ii- The stability of the molecule decreases compared to another molecule with the same bond order if the first molecule contains more anti-affinity electrons than the second molecule.



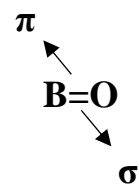
$$B=O$$

$$B.O = 9 - 4/2$$

$$= 5/2$$

$$= 2.5$$

It has a magnetic character due to the presence of a single electron (paramagnetic).



paramagnetic property.

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2p_y} = \pi_{2p_z} < \sigma_{2p_x} < \pi^*_{2p_y} = \pi^*_{2p_z} < \sigma^*_{2p_x}$$

Home work: Draw a molecular diagram of BN & CO.

Therefore, the NO^+ molecule is considered more stable than the NO molecule because the NO^+ molecule has a high effective nuclear charge. In addition, the loss of an electron from the orbital against the bond leads to an increase in the bond order from 2.5 for NO to 3 in NO^+ .

حفظ مهمة

The stability of the molecule depends on:

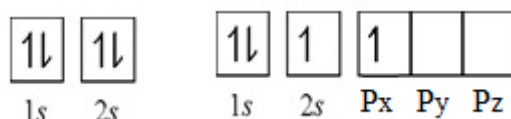
1. The higher the bond order.
2. The greater the effective nuclear charge of the molecule. (Z^*)
3. The smaller the radii of the two united atoms.
4. The greater the number of bonding electrons and the smaller the number of electrons in non-bonding orbitals.

Example: Write the electronic configuration and arrange the following molecules in order to increase stability according to molecular orbital theory (MOT) and give reason?

(CN⁻, CO, NO⁺), (CN⁻, CO⁺, BO), (NO⁺, NO⁻, NO), (O₂, O₂⁻, O₂⁼), (Be, Be₂, B₂, C₂, N₂).

Example: Draw the energy levels for the following molecules according to molecular orbital theory Na₂, F₂, Cl₂ and find the bond order and magnetic properties?

Hybridization



The formation of the compound **BeCl₂** is an indication that it is possible to transfer an electron from the **2S** secondary shell to the **2P** secondary shell to form (the excited atom) with a little energy. This can happen to form two bonds sigma type **σ** with **Be**. Each chloride atom contains an orbital, which contains one, preferably an orbital. The **P_x** is because it has a similar symmetry, which allows the formation of a sigma bond (**σ**).

As for beryllium, it contains one electron in the **2S** orbital and one electron in **2P**. If we assume that the **2S** electron of the Be atom can form a sigma bond **σ** with the **P_x** secondary orbital of the first chloride atom and another sigma bond **σ** between the secondary **Be** orbital type **2P_x** and secondary **Cl** orbital (**P_x**) For the second **Cl** atom, there will be two unequal bonds. This means that the energy of the first **BeCl** bond differs from the energy of the second **BeCl** bond, or in other words, the first bonding electron double is not equivalent to the other bonding electron double.