**Assignment No: 01**

# Assignment on Resonance, Hybrid orbitals, Valence shell and Molecular orbital.

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**Introduction:**

This assignment provides the concepts of four very important terms in chemistry. The aim of the assignment is to understand the meaning of the four terms also to understand their causes, types, effects and so many characteristics.

The first term here is **resonance** which refers to a way of describing delocalized electrons within certain molecules of polyatomic ions where the bonding cannot be expressed by a single Lewis formula.

The second one is **hybrid orbitals** which refers to the concept of mixing atomic orbitals with the same energy levels to give a degenerated new type of orbitals.

The third term is **valence shell** and it is the outermost shell of every element. Valence shell takes part to make bond between different atoms.

The forth and final one is molecular orbital. A **molecular orbital** is a [mathematical function](https://en.wikipedia.org/wiki/Function_(mathematics)) describing the location and [wave-like](https://en.wikipedia.org/wiki/Matter_wave) behavior of an [electron](https://en.wikipedia.org/wiki/Electron) in a [molecule](https://en.wikipedia.org/wiki/Molecule). This function can be used to calculate chemical and physical properties such as the probability of finding an [electron](https://en.wikipedia.org/wiki/Electron) in any specific region.

**Resonance**

Resonance is a way of describing delocalized electrons within certain molecules of polyatomic ions where the bonding cannot be expressed by a single Lewis formula. A molecule of ion with delocalized electrons is represented by several resonance structure.

**Delocalization and Resonance Structure Rules:**

1. Resonance structures should have the same number of electrons do not add or subtract any electrons.
2. Each resonance structures follows the rules of writing Lewis Structure.
3. The hybridization of the structure must stay the same.
4. The skeleton of the structure can not be changed. (only the electrons move).
5. Resonance structure must also have the same number of lone pairs.

**Types of Resonance Effects:**

Two types of Resonance effects exist, namely:

* Positive resonance effect
* Negative resonance effect

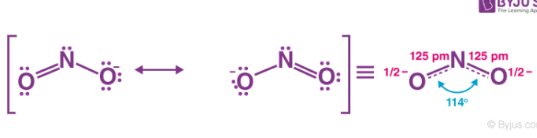
**Positive Resonance Effect:**

The positive resonance effect happens when the groups release electrons to the other molecules by the delocalization process. Usually the group are denoted by +R or +M . The molecular electron density increases in this process. The positive resonance effect examples are –OH, -OR, -SH and –SR.

**Negative Resonance Effect:**

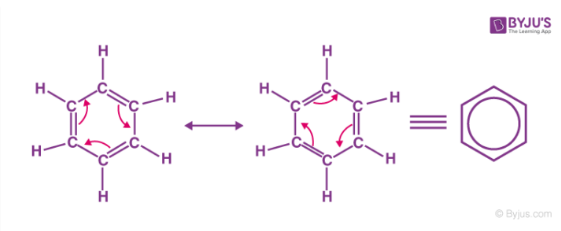
The Negative Resonance effect happens when the groups withdraw the electrons from the other molecules by the delocalization process. Usually, the groups are denoted either by –R or –M. The molecular electron density is said to decrease in this process. The negative resonance effect example are, C=O, -COOH, -C≣N, and –NO2 .

**Resonance structure of NO-2  ion:**

In the nitrite ion, the bond lengths of both nitrogen-oxygen bonds are equal. The Lewis dot structure of NO-2 highlight a difference in bond order of the two N-O bonds. The resonance hybrid of this polyatomic ion, obtained from its different resonance structures, can be used to explain the equal bond lengths, as illustrated below.

**Resonance Structure of Benzene:**

Benzene is very important aromatic hydrocarbon in organic chemistry . It has the chemical formula C6H6. The molecules of benzene have a cyclic structure consisting of alternating single and double bonds between adjacent carbon atoms. Each carbon atom is also bonded to one hydrogen atom. The two possible resonance structure of benzene are illustrated below.



**Hybrid orbitals**

**Orbital hybridisation** (or **hybridization**) is the concept of mixing [atomic orbitals](https://en.wikipedia.org/wiki/Atomic_orbital) into new *hybrid orbitals* (with different energies, shapes, etc., than the component atomic orbitals) suitable for the pairing of electrons to form [chemical bonds](https://en.wikipedia.org/wiki/Chemical_bond) in [valence bond theory](https://en.wikipedia.org/wiki/Valence_bond_theory)

**Type of Hybridization:** Based on the types of orbitals involved in mixing, the hybridization can be classified as sp3, sp3, sp, sp3d, sp3d2,sp3d3. Let us now discuss the various types of hybridization, along with their example.

**sp Hybridization:**

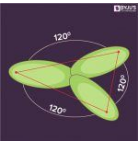
sp hybridizations is observed when one s and one p orbital in the same main shell of an atom mix the form two new equivalent orbitals. The new orbitals formed are called **sp** hybridized orbitals. It forms linear

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Examples of sp Hybridization:

* All compounds of beryllium like BeF2, BeCl2
* All compounds of carbon containing triple Bond like C2H2.

**sp2 Hybridization:** sp2 hybridization is observed when one s and two p orbitals of the same shell of an atom mix to form 3 equivalent orbital. The new orbitals formed are called **sp2Hybrid orbitals.**

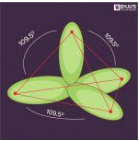


Example of sp2 Hybridization

* All the compounds of Boron i.e. BF3, BH3
* All the compounds of carbon containing a carbon- carbon double bond, Ethylene (C2H4)

**sp3Hybridization:**

When one “s” orbitals and 3 “p” orbitals belonging to the same shell of an atom mix together to form four new equivalent orbital, the type of hybridization is called tetrahedral hybridization of sp3 .



Example of sp3 hybridization : ethane (C2H4)

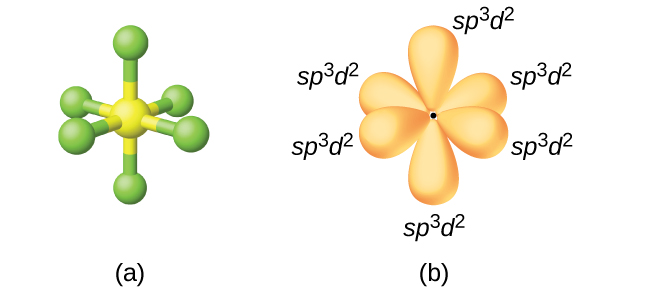
**sp3d Hybridization:** sp3d hybridization involves the mixing of 3porvitals and 1d orbitals and 1d orbitals to form 5 **sp3d**hybridized orbitals of equal energy.

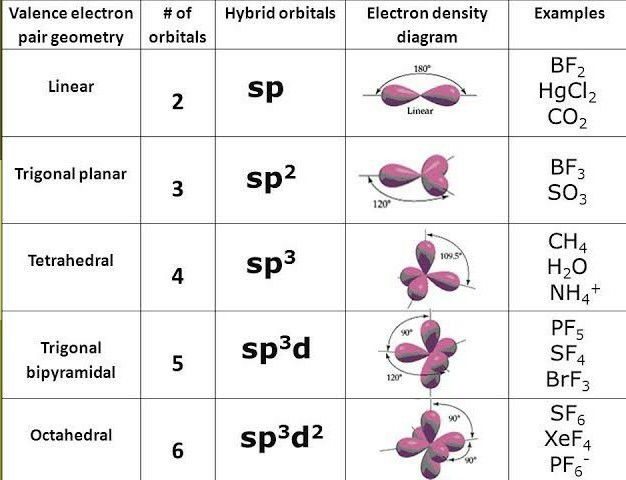
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**sp3d2hybridization;**

When one s-orbital, three p-orbitals, and two d-orbitals hybridize to give six equivalent sp3d2  **hybrid** orbitals of equal energy. This **hybridization** is called sp3d2 **hybridization**. -Properties: six equivalent sp3d2 **hybrid** orbitals are directed towards the six corners of a regular octahedron.

In SF6, one electron each from 3s and 3p orbitals is promoted to 3d orbitals The six orbitals get **hybridized** to form six sp3d2 hybrid orbitals. Each of these sp3d2 hybrid orbitals overlaps with 2p orbital of fluorine to form S–F bond. Thus, SF6 molecule has octahedral structure.



At a glance of hybridization

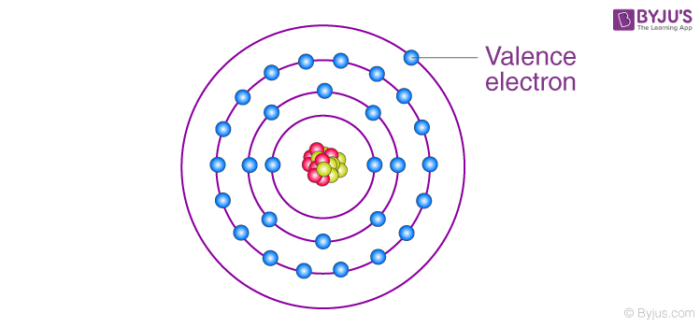
**Valence shell**

Valence shell is the outermost shell of every element. Atom of every element have different electronic configurations based on the atomic number of each element. Electronic configuration refers to the distribution of electrons in various shells/orbits/energy levels of every atom.

**Valance Electron:**

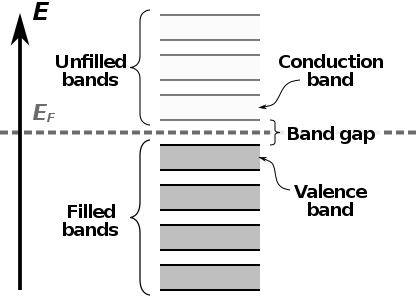
a **valence electron** is an outer shell **electron** that is associated with an atom, and that can participate in the formation of a chemical bond if the outer shell is not closed; in a single covalent bond, both atoms in the bond contribute one **valence electron** in order to form a shared pair.

|  |  |
| --- | --- |
| Periodic table | valence electron |
| Group (I) | 1 |
| Group (II) | 2 |
| group 13 (III) | 3 |
| group 14 (IV) | 4 |
| group 15 (V) | 5 |
| group 16 (VI) | 6 |
| group 17 (VII) | 7 |
| group 18(VIII) | 8 |



**Valence band:**

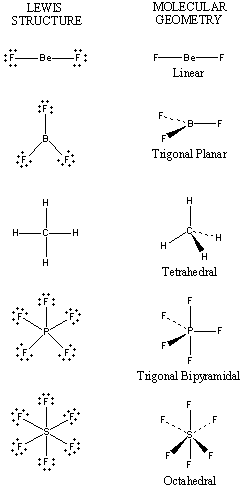
The **valence band** is the **band** of electron orbitals that **electrons** can jump out of, moving into the **conduction band** when excited. The **valence band** is simply the outermost electron orbital of an atom of any specific material that **electrons** actually occupy. This is closely related to the idea of the **valence** electron



**Valence-Shell Electron-Pair Repulsion Theory (VSEPR)**

**Predicting the Shapes of Molecules**

There is no direct relationship between the formula of a compound and the shape of its molecules. The shapes of these molecules can be predicted from their Lewis structures, however, with a model developed about 30 years ago, known as the **valence-shell electron-pair repulsion (VSEPR) theory**.

The VSEPR theory assumes that each atom in a molecule will achieve a geometry that minimizes the repulsion between electrons in the valence shell of that atom. The five compounds shown in the figure below can be used to demonstrate how the VSEPR theory can be applied to simple molecules.

There are only two places in the valence shell of the central atom in BeF2 where electrons can be found. Repulsion between these pairs of electrons can be minimized by arranging them so that they point in opposite directions. Thus, the VSEPR theory predicts that BeF2 should be a **linear**molecule, with a180o angle between the two Be-F bonds.



There are three places on the central atom in boron trifluoride (BF3) where valence electrons can be found. Repulsion between these electrons can be minimized by arranging them toward the corners of an equilateral triangle. The VSEPR theory therefore predicts a **trigonal planar** geometry for the BF3 molecule, with a F-B-F bond angle of 120o.



BeF2 and BF3 are both two-dimensional molecules, in which the atoms lie in the same plane. If we place the same restriction on methane (CH4), we would get a square-planar geometry in which the H-C-H bond angle is 90o. If we let this system expand into three dimensions, however, we end up with a **tetrahedral**molecule in which the H-C-H bond angle is 109o28'.



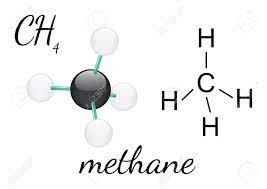
Repulsion between the five pairs of valence electrons on the phosphorus atom in PF5 can be minimized by distributing these electrons toward the corners of a **trigonal bipyramid**. Three of the positions in a trigonalbipyramid are labeled *equatorial* because they lie along the equator of the molecule. The other two are *axial* because they lie along an axis perpendicular to the equatorial plane. The angle between the three equatorial positions is 120o, while the angle between an axial and an equatorial position is 90o.



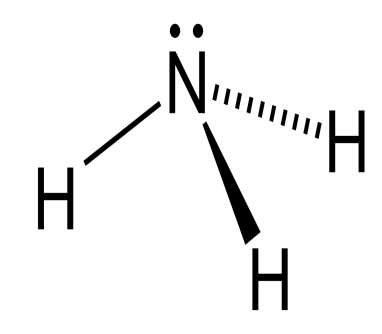
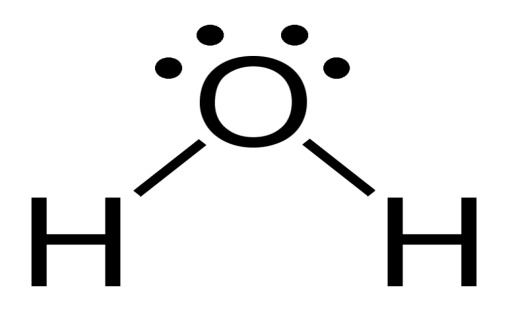
There are six places on the central atom in SF6 where valence electrons can be found. The repulsion between these electrons can be minimized by distributing them toward the corners of an **octahedron**. The term *octahedron* literally means "eight sides," but it is the six corners, or vertices, that interest us. To imagine the geometry of an SF6 molecule, locate fluorine atoms on opposite sides of the sulfur atom along the *X*, *Y*, and *Z* axes of an *XYZ* coordinate system.



Another important behavior of electrons of valence shell is that it causes distorted geometrical shape of the molecules. When the central atom is surrounded by bond pair only it gives the symmetrical shape to the molecules. For example we can mention methane(CH4). The angle is 109.5˚.

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Then if the central atom is surrounded by bond pair as well as lone pair, the molecule gets a distorted geometrical shape. For example NH3 ,H2O molecules. The bond angles are respectively 107˚ and 104.5˚.

As the number of lone pair electron increases the bond angle decreases and the molecules get more distorted. There is a sequence of repulsion between bond pair and lone pair electrons i.e. **L.p-L.p> L.p-B.p >B.p-B.p.**

Molecular orbital

In [chemistry](https://en.wikipedia.org/wiki/Chemistry), a **molecular orbital** is a [mathematical function](https://en.wikipedia.org/wiki/Function_(mathematics)) describing the location and [wave-like](https://en.wikipedia.org/wiki/Matter_wave) behavior of an [electron](https://en.wikipedia.org/wiki/Electron) in a [molecule](https://en.wikipedia.org/wiki/Molecule). This function can be used to calculate chemical and physical properties such as the probability of finding an [electron](https://en.wikipedia.org/wiki/Electron) in any specific region.

In an isolated [atom](https://en.wikipedia.org/wiki/Atom), the orbital electrons' location is determined by functions called [atomic orbitals](https://en.wikipedia.org/wiki/Atomic_orbital). When multiple atoms combine chemically into a [molecule](https://en.wikipedia.org/wiki/Molecule), the electrons' locations are determined by the molecule as a whole, so the atomic orbitals combine to form molecular orbitals.

the electrons in isolated atoms as having certain spatial distributions, called orbitals, each with a particular orbital energy. Just as the positions and energies of electrons in atoms can be described in terms of atomic orbitals (AOs), the positions and energies of electrons in molecules can be described in terms of molecular orbitals (MOs) A particular spatial distribution of electrons in a molecule that is associated with a particular orbital energy.—a spatial distribution of electrons in a molecule that is associated with a particular orbital energy. As the name suggests, molecular orbitals are not localized on a single atom but extend over the entire molecule.

Formation of molecular orbitals

Molecular orbitals arise from allowed interactions between [atomic orbitals](https://en.wikipedia.org/wiki/Atomic_orbital), which are allowed if the symmetries (determined from [group theory](https://en.wikipedia.org/wiki/Group_theory)) of the atomic orbitals are compatible with each other. Efficiency of atomic orbital interactions is determined from the [overlap](https://en.wikipedia.org/wiki/Orbital_overlap) (a measure of how well two orbitals constructively interact with one another) between two atomic orbitals, which is significant if the atomic orbitals are close in energy. Finally, the number of molecular orbitals formed must be equal to the number of atomic orbitals in the atoms being combined to form the molecule.

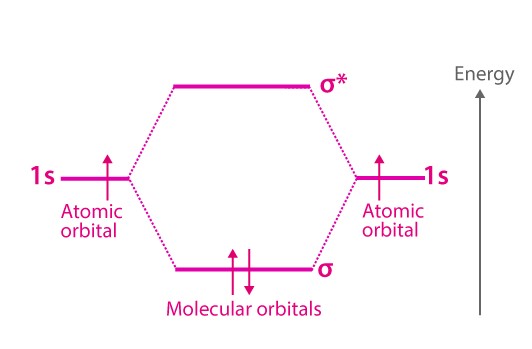
## Molecular Orbital Theory:

The Molecular Orbital Theory (often abbreviated to MOT) is a theory on chemical bonding to describe the structure and properties of different molecules. In simple terms, the molecular orbital theory states that each atom tends to combine together and form molecular orbitals. As a result of such arrangement, electrons are found in various atomic orbitals and they are usually associated with different nuclei. The valence-bond theory failed to adequately explain how certain molecules contain two or more equivalent bonds whose bond orders lie between that of a single bond and that of a double bond, such as the bonds in resonance-stabilized molecules. This is where the molecular orbital theory proved to be more powerful than the valence-bond theory (since the orbitals described by the MOT reflect the geometries of the molecules to which it is applied).

The key features of the molecular orbital theory are listed below.

* The total number of molecular orbitals formed will always be equal to the total number of atomic orbitals offered by the bonding species.
* There exist different types of molecular orbitals viz; bonding molecular orbitals, anti-bonding molecular orbitals, and non-bonding molecular orbitals. Of these, anti-bonding molecular orbitals will always have higher energy than the parent orbitals whereas bonding molecular orbitals will always have lower energy than the parent orbitals.
* The electrons are filled into molecular orbitals in the increasing order of orbital energy (from the orbital with the lowest energy to the orbital with the highest energy).
* The most effective combinations of atomic orbitals (for the formation of molecular orbitals) occur when the combining atomic orbitals have similar energies.

Molecular orbital theory approximation of the molecular orbitals as linear combinations of atomic orbitals can be illustrated as follows.



Bond Order in Molecular Orbital Theory:

In the Lewis electron structures, the number of electron pairs holding two atoms together was called the bond order. In the molecular orbital approach, bond order One-half the net number of bonding electrons in a molecule. is defined as one-half the net number of bonding electrons:

To calculate the bond order of H2  according to MOT we see that the bonding molecular orbital contains two electrons, while the  antibonding molecular orbital is empty. The bond order of H2 is therefore

=1

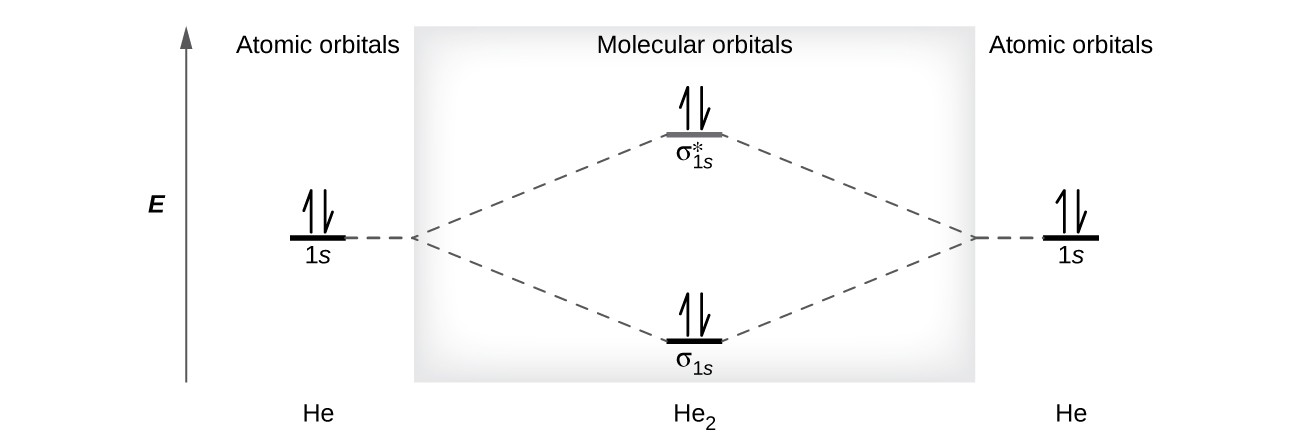
This result corresponds to the single covalent bond predicted by Lewis dot symbols. Thus molecular orbital theory and the Lewis electron-pair approach agree that a single bond containing two electrons has a bond order of 1. Double and triple bonds contain four or six electrons, respectively, and correspond to bond orders of 2 and 3.

Now using the energy level diagrams the possible bond order of different molecules are given below.

1. **Bond order** **0**:

The bond order zero means there exists no bond between two atoms. Such a example we can mention **He-He** bond.

From the figure we can see that

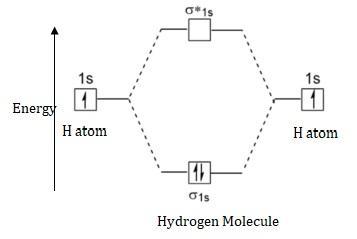


the bond order of **He-He** is , = . So we can say that **He-He** does not exist as the bond order of the molecule is **0**.

1. **Bond order 1** :

Bond order 1 means there is a single bond between two atoms.For example we can mention **H2** **(H-H).**

From the figure we get that

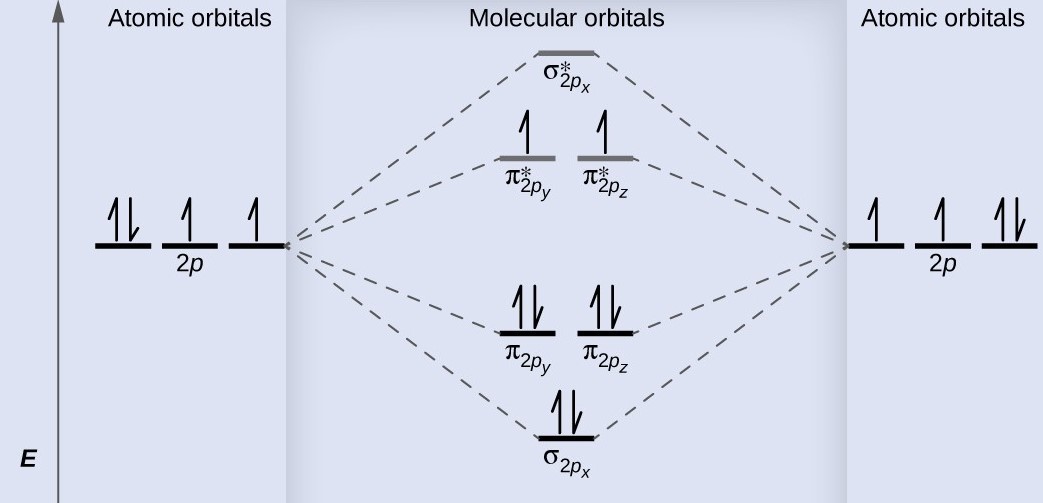


the bond order is, .So we can say that there is a single bond between two hydrogen atoms.

1. **Bond order 2:**

Bond order 2 means there exists double bonds between two atoms.

For example we can mention here **O2 (O=O)** molecules.From the figure we get ,

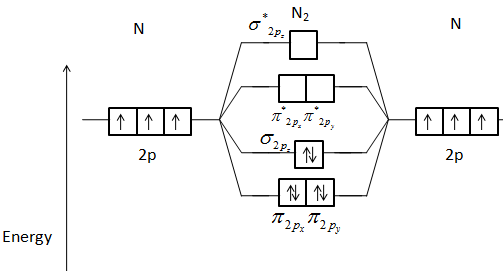


The bond order is, . So we can say that there exists double bonds between two oxygen atoms.

1. **Bond order 3:**

Bond order 3 means there exists triple bonds between two atoms.

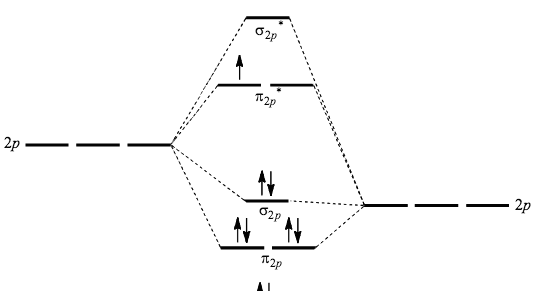
For example we can mention here **N2 (N ≡ N)** molecules.From the figure we get ,

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The bond order is,

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So we can say that there exists triple bonds between two nitrogen atoms.

Another special thing we get from the energy level diagrams is the magnetic behavior of molecules. Considering NO molecule, we can see from the figure 

N NO O

Here we see that there is a odd(single) electron in the antibonding orbital which reveals the paramagnetic behavior of the NO molecule.

**Conclusion :**

The discussion above about all the terms mentioned in the introduction portion. From the discussion we get the different kind of knowledge about resonance, hybridization, valence shell and molecular orbitals. From the discussion we can say due to resonance i.e. movement of pi electrons some elements show colorful characteristics. The hybridization tells the shape of the molecules. From the valence shell electron we can determine the group number and valence electron tells us the tendency to make bond with others. From the VSEPR theory we get the information to compare the original shape and the distorted shape of molecules of same hybridization. The molecular orbital tells us about the shared or exchanged electrons of the molecules. It also tells us about the bond order i.e. how many bonds exist between two atoms. And from this bond order we gets the information about the strength of the bond between atoms of a molecule**.**

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