Unit -03

Theories of Covalent Bonding and Shapes of Molecules

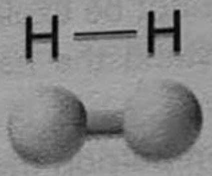
After reading this unit, the students will be able to:

- Use VSEPR and VBT theories to describe the shapes of simple covalent molecules. (Applying)
- Describe the features of sigma and pi bonds. (Understanding)
- Describe the shapes of simple molecules using orbital hybridization. (Applying)
- Determine the shapes of some molecules from the number of bonded pairs and lone pairs of electrons around the central atom. (Analysing)
- Define bond energies and explain how they can be used to compare bond strengths of different chemical bonds. (Analysing)
- Predict the molecular polarity from the shapes of molecules. (Applying)
- Describe how knowledge of molecular polarity can be used to explain some physical and chemical properties of molecules. (Analysing)
- Describe the change in bond lengths of hetero-nuclear molecules due to difference in electronegativity values of bonded atoms. (Understanding)
- Describe the difference among molecular, network and metallic solids. (Understanding)
- Explain what is meant by the term ionic character of a covalent bond. (Understanding)

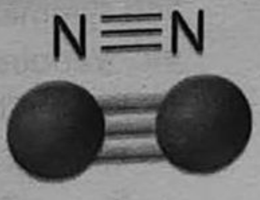
Teaching
12

Assessment
01

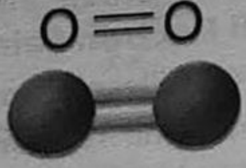
Weightage %
11



Single bond



Triple bond



Double bond

Introduction

Dalton's atomic theory opened the ways for the scientists to think abou nature of forces that hold the atoms together. Earlier the scientists assumed chemical bond result from attraction between oppositely charged particles. S molecules like N_2, H_2 and other organic compounds were discovered which coul be explained on the basis of this concept.

In 1916, G.N. Lewis proposed that the sharing of electron was respons for the formations of bonds between molecules. He used electronic configurat to explain that how atoms join together to form molecules. He gave electronic theory of valence, according to this theory, *In chemical bond format atoms interact by sharing of electrons, to attain noble gas electr configuration.* This theory was called doublet or octet theory. This the described the sharing of electron, and covalent bond formation. This theory a identified the single, double and triple covalent bonds by sharing of one, two a three pairs of electrons respectively. The electronic theory of valence tells ab the number of electrons present in the valence shell of the central at However, this theory fails to explain geometry of molecules.

You have studied in the previous grades about the chemical bonding a its different types. In this unit, you will learn about the shapes of molecu physical and chemical properties of molecules, molecular polarity and bo energies.

3.1 Shapes of Molecules

The shape of molecules can be determined in the laboratory by mo methods such as X–rays diffraction and electron diffraction techniques. Molec shapes are important because they provide information about molecular po and symmetry. The shape of molecule cannot be explained by the covalent bo etc. Various theories are used to understand the nature of bond and shap molecule. These theories are,

i. The valence shell electron pair repulsion theory (VSEPR)
ii. The valence bond theory
iii. The molecular orbital theory

3.1.1 Valence Shell Electron Pair Repulsion Theory (VSEPR)

In 1970, R. G. Gillespie and Nyholm proposed a theory known as Valence shell electron pair repulsion or VSEPR theory. This theory is base electron pair repulsion in valence shell of central atom. This theory states that *electron pairs (both lone pairs and shared pairs) surrounding the central ato* *be arranged in space as far apart as possible to minimize the electrostatic repulsion between them.* This theory helps in determining the geometries of the molecules. The main postulates are,

1. Pairs of electrons are arranged in space around the central atom in such a way that the distance between them is maximum and electron pair repulsion is minimum.
2. These electron pairs which form bonds are called bond pairs and those electron pairs, which do not form bonds, are called lone – pairs.
3. A lone pair of electrons is capable of occupying more space on the central atom than a bond pair. Hence, it will cause more repulsion as compared to bond pair. The electron pairs repulsion decrease in the following order,

   Lone pair – Lone pair > Lone pair – Bond pair > Bond pair – Bond pair
4. Forces of repulsion decrease with increasing bond angles.
5. As multiple covalent bonds and lone pair of electrons, occupy more space than the bond pairs, therefore, the ideal bond angles are changed.
6. Multiple bonds behave as a single electron pair bond in structural determination.
7. The effect of a bonding electron pair decreases with increasing electronegativity of an atom bonded to central atom forming in a molecule.
8. Shapes of molecules depend upon the number and nature of the electron pairs in space around the central atom.

Applications of VSEPR theory

Covalent bond is directional in nature. It explains the geometry of the molecules and tells about the possible structure of the molecule. Examples are,

Reading Check

Write down at least five postulates of the VSEPR theory.

1. Shapes of Molecules Containing Two Electron Pairs

Beryllium chloride ($BeCl_2$) is a typical example of molecules, which contain two electron pairs. Itś Lewis structure is given below.

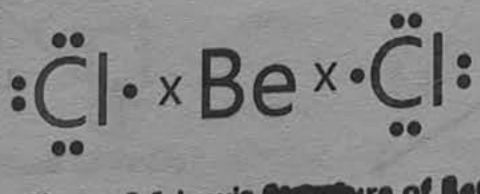


Figure 3.1 Lewis [illegible]ure of $BeCl_2$

Two bond pairs are present in valence shell of the central beryllium atom, which are arranged in such a way that minimizes the repulsion between them.

The bonding pair will occupy the opposite side of the beryllium, forming an ang of 180°. This angle gives linear structure to $BeCl_2$ or a straight line arrangement the atoms. Therefore, $BeCl_2$ molecule is **linear**.

Linear Structure of $BeCl_2$ VSEPR model of $BeCl_2$

Figure 3.2

2. Shapes of Molecules Containing Three Electron Pairs

a) All three are Bond Pairs

Example is, Boron tri-fluoride (BF_3)

Boron, B_5 = $1s^2$, $2s^2$, $2p_x^1$, $2p_x^0$, $2p_z^0$

has three valence electrons.

The boron has three valence electrons; all these three electrons form three bonds and no unshared electrons are left. The three bond pairs will be at maximum distance from each other. Therefore, the repulsion between them is minimum and the distance is maximum. The Lewis structure of BF_3 is shown in figure 3.3.

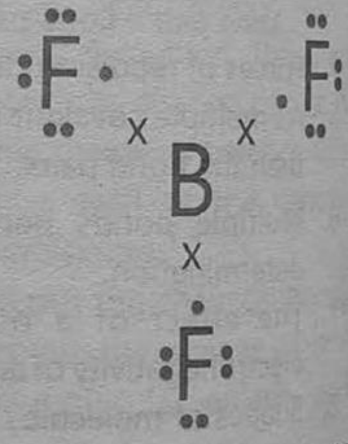
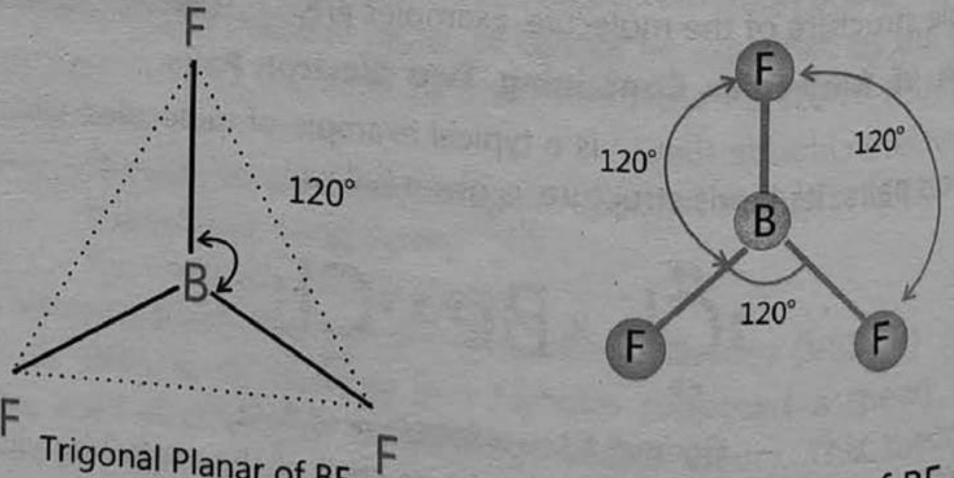


Figure 3.3 Lewis Structure of BF_3

The three F atoms will occupy the corners of an equilateral triangle. All th four atoms (three F and one B) lie in the same plane. The angle between them is 12 The shape of such molecule is **trigonal planar.**



Trigonal Planar of BF_3 VSEPR Model of BF_3

Figure 3.4

Tidbit

Many boron compounds are electron-deficient, meaning that they lack an octet of electrons (mostly have six electrons) around the central boron atom. This deficiency of electron is responsible for acidic nature of boron compounds.

b. Two Bond Pairs and One Lone Pair

Example of the molecules having two bond pairs and one lone pair is,
Stannous Chloride ($SnCl_2$)

Stannom, Sn_{50} = [Kr] $4d^{10}5s^25p^2$ has four valence electrons. Two electrons present in 5s orbital remain non-bonding (lone pair) and two electrons of 5p orbitals form two covalent bonds with chlorine atoms. The Lewis structure of $SnCl_2$ is,

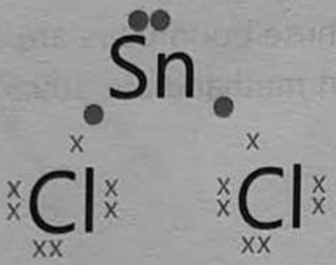


Figure 3.5 Lewis Structure of $SnCl_2$

Molecules with two bond pair electrons and one lone pair shall have the non – linear geometry. The lone pair occupies more space than the bond pair of electrons. Therefore, it pushes the bond pairs of electrons. The lone pair present in the stannous chloride occupies one corner of the triangle and the other two are occupied by two Cl atoms as shown in figure 3.6. Therefore, the bond angle is reduced than ideal angle of 120°. The effective molecular shape of $SnCl_2$ is angular (V-Shaped).

Angular structure of $SnCl_2$

VSEPR Model of $SnCl_2$

Figure 3.6

3. Shapes of Molecules Containing Four Electron Pairs

i. All the four are Bond Pairs

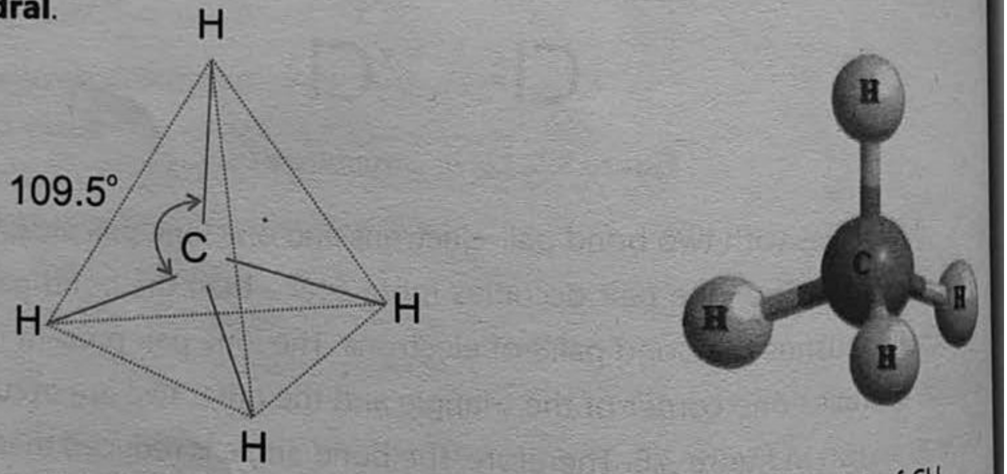
Example of molecules having four bond pairs in valence shell of central atom is,

Methane (CH_4)

Carbon has four electrons ($1s^2$, $2s^2$, $2p_x^1$, $2p_y^1$, $2p_z^0$) in the valence shell, which share with four electrons of four hydrogen atoms. All the four pairs are bond pairs.

Figure 3.7 Lewis Structure of C

The electron pairs are arranged in such a manner that the repulsion is minimum and the distance is maximum. These bond pairs are arranged in tetrahedral manne The H – C – H bond angles in methane are 109.5°and the shape of the molecu is **tetrahedral**.



Tetrahedral Structure of CH_4

VSEPR Model of CH_4

Figure 3.8

ii. Three Bond Pairs and One Lone Pair

Example of molecules having three bond pairs and one lone pair in valen shell of central atom is,

Ammonia (NH_3)

The nitrogen, $N_7 = (1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1)$ has five electrons in valence shell. In NH_3 molecule has four electron pairs in the valence shell of central atom. Three of them are bond pairs and one is lone pair.

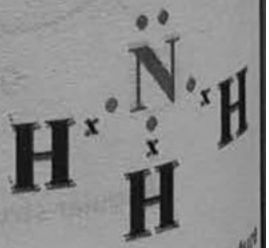
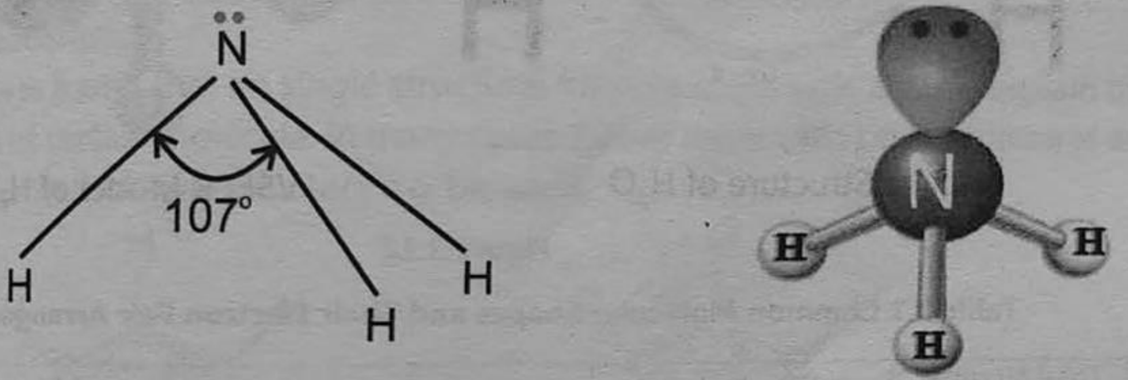


Figure 3.9 Lewis Structure of NH_3

The electron pairs are arranged in such a manner that the repulsion between them is minimum and the distance is maximum.

According to VSEPR theory, lone pair – bond pair repulsion is greater than bond pair – bond pair repulsion. The lone pair occupies more space than the bond pair of electrons. Therefore, the three N – H bond pairs are pushed closer and bond angle decreases. Therefore, the ideal bond angle is changed and reduced to 107.5°. Moreover, due to absence of atom on lone pair, NH_3 does not show the expected tetrahedral arrangement but possesses a **trigonal pyramidal** structure with the observed angle 107.5°as shown in figure 3.10.



Trigonal Pyramidal Structure of NH_3

VESPR Model of NH_3

Figure 3.10

iii. Two Bond Pairs and Two Lone Pairs

Example of the molecules having two bond pairs and two lone pairs in the valence shell of central atom is water.

Water (H_2O)

The oxygen, $O_8 = (1s^2, 2s^2, 2p_x^2, 2p_y^1, 2p_z^1)$, in water molecule has four electron pairs; two bond pairs and the two lone pairs. The lone pair – lone pair repulsion is maximum as compared to bond pair – bond pair repulsion, resulting in the decrease of H – O – H bond angle to 104.5°. The electron pairs are arranged in such a manner that the repulsion between them is minimum and the distance is maximum.

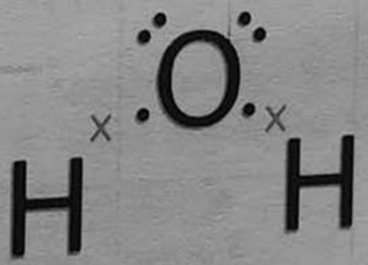
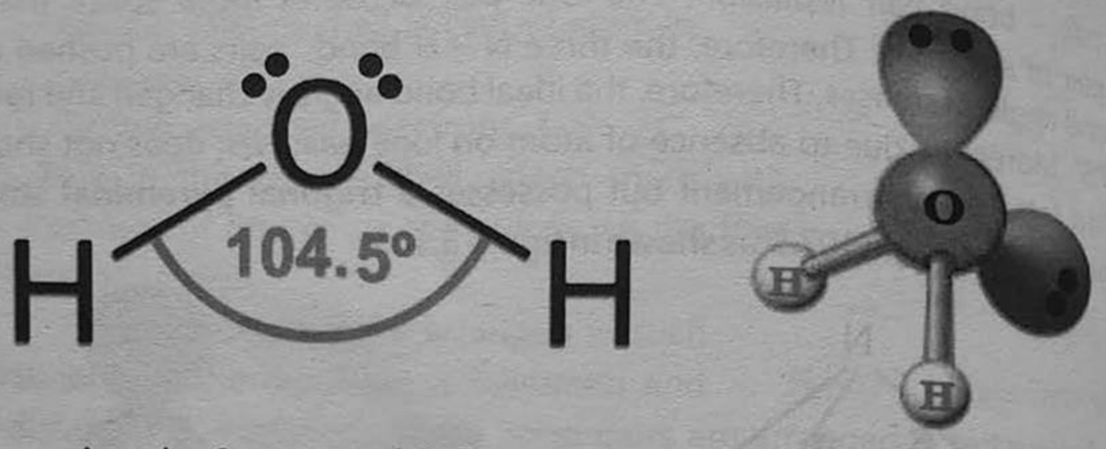


Fig: 3. 11 Lewis Structure of H_2O

Molecules with four electron pairs repel each other and thus are directed towards the four corners of a regular tetrahedron. However, the two lone pairs of electrons occupy more space than the bond pair of electrons. Therefore, they push the bond pairs of electrons to greater extent. Thus, the ideal bond angle is reduced. Moreover, due to absence of atoms on lone pair, the H_2O molecule is bent at an angle of 104.5°. Such a molecule is called a bent molecule (V – shaped) or angu molecule.

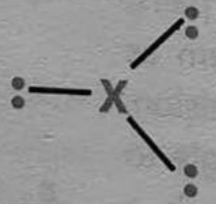
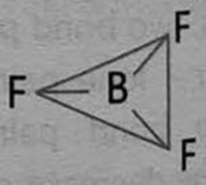
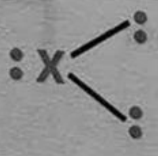
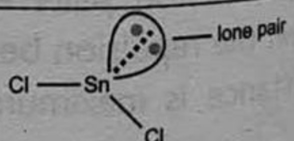
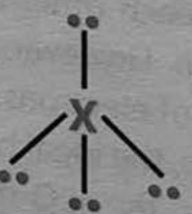
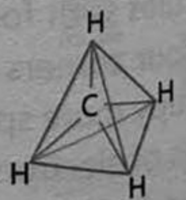


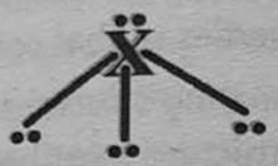
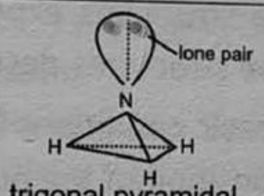
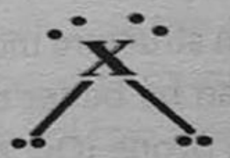
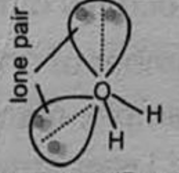
Angular Structure of H_2O

VSEPR Model of H_2O

Figure 3.12

Table 3.1 Common Molecular Shapes and Their Electron Pair Arrangements

Total Number of electron pairs Present in Valence Shell of Central Atom	Geometric arrangements of electron pairs	Type of electron pairs	Name of molecular shape	Example
2	:—X—:	2 bond pair 0 lone pair	Cl—Be—Cl linear	$BeCl_2$
3		3 bond pair 0 lone pair	 trigonal planar	BF_3
3		2 bond pair 1 lone pair	 angular (Bent)	$SnCl_2$
4		4 bond pair 0 lone pair	 tetrahedral	CH_4

4		3 bond pair 1 lone pair	 trigonal pyramidal	NH_3
4		2 bond pair 2 lone pair	 angular (Bent)	H_2O

3.1.2 Resonance

It was found that no single structural formula could satisfactorily explain the structures of certain molecule. In many cases, two or more valid Lewis structures are used to show a molecule structure e.g. benzene.

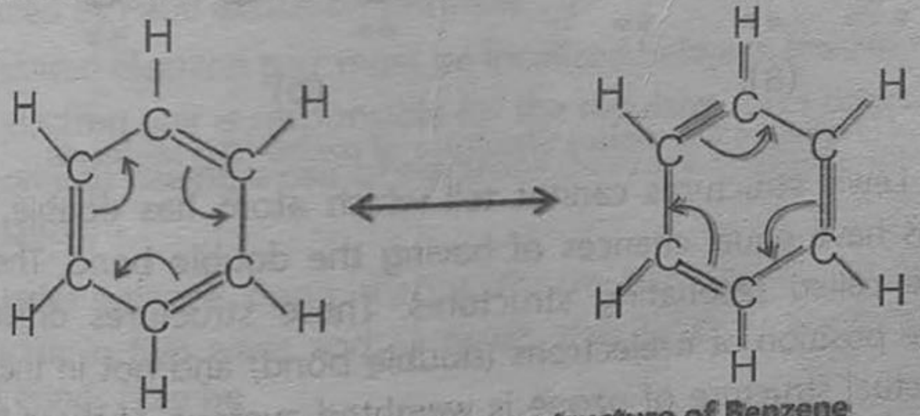


Figure 3.13 Resonance structure of Benzene

Even though these Lewis structures differ in the position of their electrons, they all represent the same molecule. It is important to know that none of these Lewis structures has a real physical existence, and the best representative is certainly the weighted average of these Lewis structures.

The phenomenon in which two or more structures can be written for a compound, which involves identical positions of atom, is called resonance. In other words, you can simply say that, a molecule or ion that has multiple correct Lewis structures shows resonance. Each of these Lewis structures is called a resonating structure. The actual structure of the molecule is said to be a resonance hybrid of all possible structures.

This led to the idea that such molecules exist in the state, which is combination of two or more electronic structures.

Tidbit

Resonance Hybrid

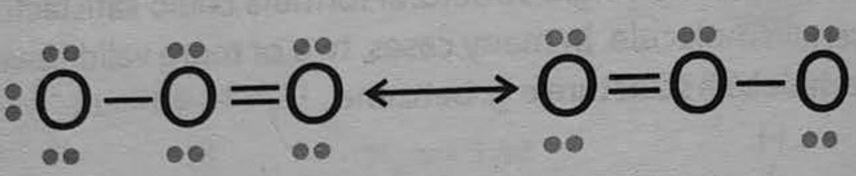
The weighted average of resonance contributors, which best represents, the reality. Demonstrating the molecule the way it is observed in lab.

These structures express some of the properties of the compounds b none of these structures describing all the properties of that compound.

a. The basic conditions for writing the resonating structures are,
b. The position of the nuclei (atom) in all structure must be the same.
c. The structures differ only in the position of pi(π)electrons

The number of unpaired electrons in each structure must be the same.

For example, many bonding situations can be better described with mor than one valid Lewis structure for ozone (O_3). In ozone (O_3), the central atom ha a single bond with one oxygen atom and a double bond with other oxygen ato as,



(a) (b)

Figure 3.14 Resonance Structure of ozone (O_3) Molecule

These Lewis structures cannot tell which atom has double bond. Bot oxygen atoms have equal chances of having the double bond. These possib structures are called resonating structures. These structures differ from o another in the position of π-electrons (double bond) and not in the position o atoms. The actual structure of ozone is weighted average of these two possib Lewis structures.

The phenomenon of resonance explained a number of facts, which w not explained by the simple Lewis structures. The most important effect o resonance is that it stabilizes the resonance hybrid. The energy of resonance hyb is lower than calculated value of resonating structures.

3 .2 Theories of Covalent Bonding

The following two theories are used to understand the nature of covale bond, in addition to VESPR and Resonance Theories.

1. The Valence Bond Theory (VBT) and Hybridization Theory
2. The Molecular Orbital Theory (MOT)

3.2.1 Valence Bond Theory (VBT) and Hybridization

For a theory to be accepted, it must explain experimental data and be abl predict behaviour of a substance. For example, VSEPR theory has gained widespr acceptance because it explains and predicts all dimensional molecular shapes (2D and 3D) that are consistent with experimental data collected for thousands different molecules. However, VSEPR theory does not provide an explanation of chemical bonding (sharing of electrons between atoms).

Valence bond theory is successful in explaining the sharing of electrons between atoms, bond lengths and shapes of covalent molecules. This theory was developed by W. Heitler and F. W. London in 1927.

The following are the assumptions of valence bond theory,

1. A covalent bond is formed by the overlap of half filled orbitals (have one electrons only) of two atoms.
2. If two half filled orbitals overlap, a single covalent bond is formed. If more than two half filled orbitals overlap, then multiple covalent bonds are formed.
3. The orbitals, which overlap, must have electrons with opposite spin as required by Pauli exclusion principle.
4. The shared electron pair must be localized between the atoms.
5. The electron pair is responsible for the repulsive force between atoms.
6. The orbitals having a pair of electrons (two) are unable to take part in the bond formation.

Under valence bond theory, the mutual sharing of electrons between atoms occur in two ways and as result, two types of bonds are formed. These covalent bonds may be

i. Sigma (σ) bond
ii. Pi (π) bond

i. Sigma (σ) Bond

It is formed by the linear overlap of half filled atomic orbitals. This type of overlap is maximum and hence forms a strong bond. In sigma bond, the electronic density is maximum in between the two bonded nuclei. The shared pair of electrons is attracted by two nuclei and, as a result, a decrease in energy occurs. *The bond, which is formed by the linear (head on) overlap is called sigma bond.* All single covalent bonds are sigma bonds.

The following types of overlapping result in sigma bond formation.

a) s – s overlap
b) s – p overlap
c) p – p overlap

a. s – s overlap

In this overlap, the 's–orbital' of one atom overlaps with the 's– orbital' of the other atom. For example, hydrogen molecule (H_2).

Hydrogen molecule is formed between two hydrogen atoms by ove two 1s orbitals. When two half filled, $1s^1$ orbitals of hydrogen come clos overlap each other, the energy decreases, reaches to a minimum and a sig covalent bond is formed as shown in figure 3.15.

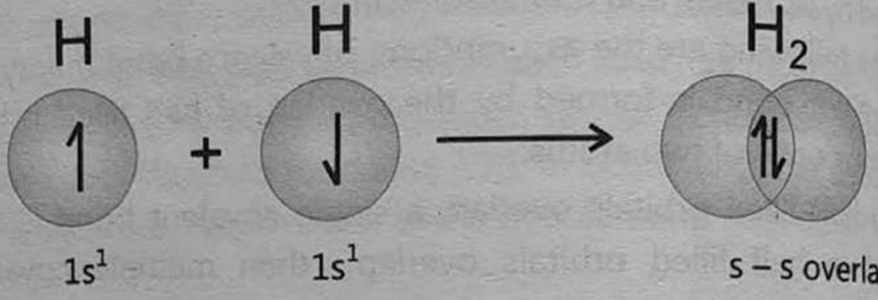


Figure 3.15 s – s Overlap in Hydrogen Orbitals

b. s – p overlap

In this overlap the 's – orbital' of one-atom overlaps with the 'p – orbital' other atom, for example, hydrogen chloride (HCl) molecule.

In HCl molecule, hydrogen contains one-half filled 1s atomic orbital there is one half filled p-atomic orbital in chlorine. When hydrogen and chl atoms come closer to one another, their '1s' and 3p orbitals overlap linearly energy decreases, reaches to a minimum and a sigma (σ) covalent bond is form shown in figure 3.16.

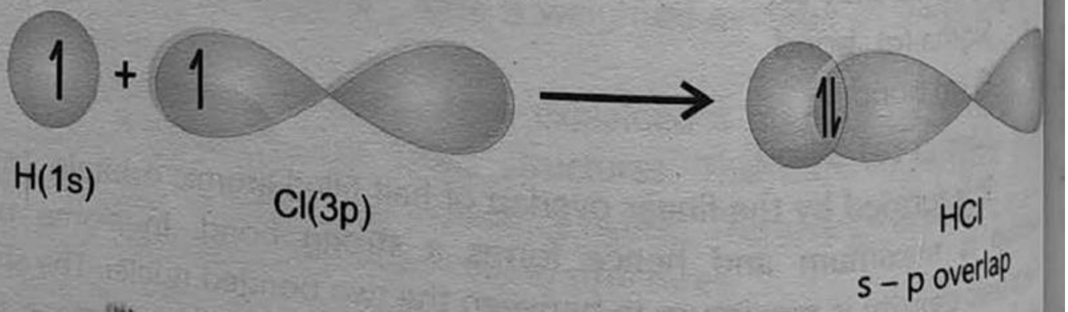


Figure 3.16 s – p Overlap in Hydrochloric Acid (HCl) Molecule

c. p – p Linear overlap

In this overlap, the 'p' orbital of one atom overlaps with another 'p' o of the other atom endwise, linearly or heads – on. In this overlapping, a s bond is formed. For example, F_2, Cl_2, Br_2

The formation of F_2 molecules is an example of p – p orbital overlap fluorine atom contains one-half filled p atomic orbital. These two half fille orbitals overlap linearly to form a sigma bond. The electronic density is max along the bond axis as shown in figure 3.17.

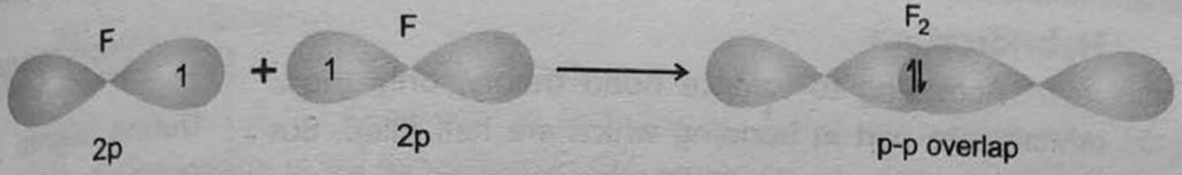


Figure 3.17 p – p Linear Overlapping in Fluorine Molecule

ii. Parallel overlap or Pi (π) Bond

The bond, which is formed by side wise or parallel overlap of the half filled p - orbitals of two already bonded atoms (through sigma bond), is called pi(π) Bond.

Pi – bond is always formed by the side wise or lateral overlap of half filled p - orbitals only. The pi – bond is weak bond. It cannot exist without the sigma bond. In pi (π) bond the orbital has two regions of electronic cloud density i.e. above and below the bond axis; unlike in sigma bond where electronic density has only one region around bond axis. Since this overlap is not maximum overlap therefore, pi bond is weaker than sigma bond.

For example, in O_2 molecule, each oxygen atom has electronic configuration $1s^2$, $2s^2$, $2p_x^2$, $2p_y^1$, $2p_z^1$. There are two half-filled p orbitals on each oxygen atom. The two oxygen atoms are joined by two bonds. One of them is formed by linear overlap of p orbitals, forming a sigma bond, while the other p – orbitals overlap side wise to form a Pi bond as shown in the figure 3.18.

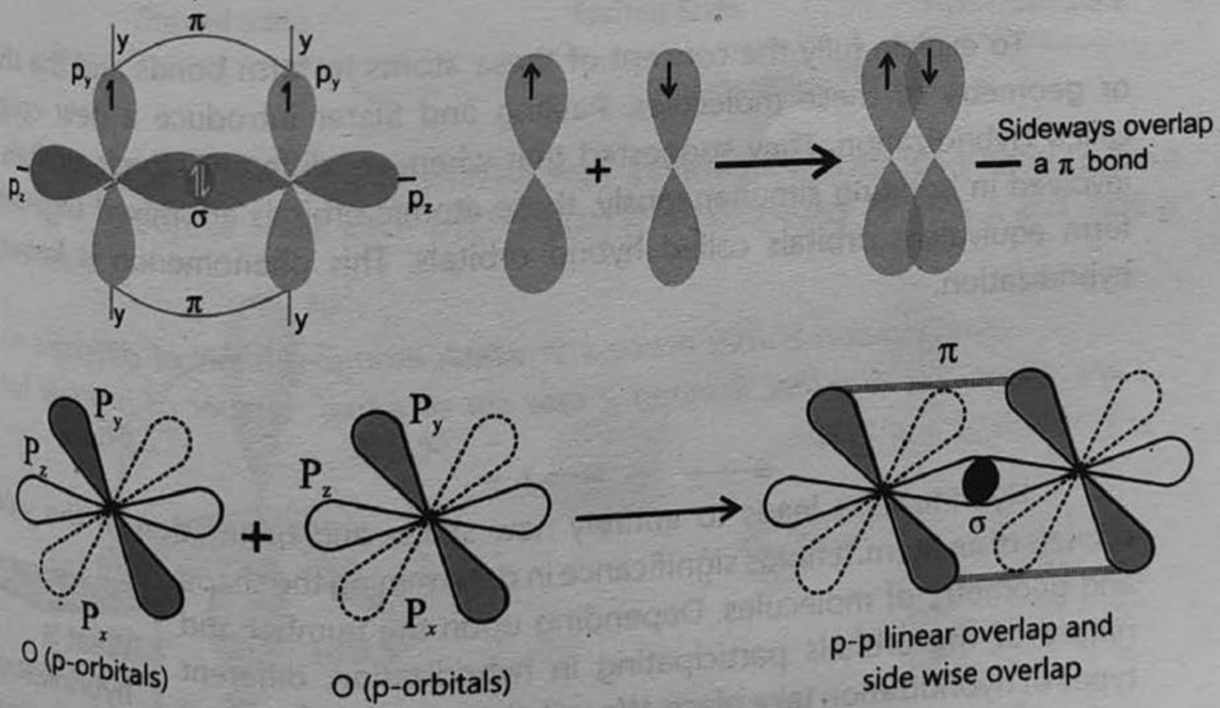


Figure 3.18 p-p Sidewise Overlap in Oxygen Molecule

Hybridization

According to valence bond theory, only those orbitals take part in bonding which are half filled. But there are molecules in which the number of bonds formed by an atom is more than their available half filled orbitals. Carbon has six electrons, $1s^2$, $2s^2$, $2p_x^1$, $2p_y^1$, $2p_z^0$. Electro configuration shows that there are only two half-filled orbitals, it is expected t only two single bonds will be formed. However, carbon atom forms four bon with other atoms in most molecules such as in CH_4 molecule.

ReadingCheck

Define sigma and pi bonds.

It is assumed that one of the 2s electrons in ground state is promoted to t empty p orbital. This new state of carbon is called the excited state.

C (Ground state) = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0$

C (Excited state) = $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$

As there are four half-filled orbitals in the carbon atom in its excited state, it expected that four bonds will be formed. The three C–H bond would be formed b the overlap of the p-orbital and 1s orbital of each hydrogen atoms. The fourth C- bond will be formed by the overlap of 2s orbital of carbon with the 1s orbital of hydrogen atom. This implies that two different type of C–H bonds are involved in th formation of methane molecule. However, experimental data shows that all the C- bonds are identical.

To explain fully the concept of these atoms to form bonds and the shap or geometry of these molecules, Pauling and Slater introduce a new concep called Hybridization. They suggested that whenever different atomic orbitals ar involved in bonding simultaneously, these atomic orbitals are mixed together t form equivalent orbitals called hybrid orbitals. This phenomenon is known a hybridization.

Hybridization is that process in which atomic orbitals of different energ and shape mix together forming a new set of equal number of orbitals having same energy and shape.

Hybridization leads to entirely new shape and orientation of the valenc orbitals of an atom. It holds significance in determining the shape and geometry of molecules. Depending upon the number and nature of the orbitals participating in hybridization, different types of hybridization take place. We will discuss only sp^3, sp^2 and sp hybridization.

Reading Chec

What is hybridization?

i. sp^3 Hybridization

The mixing of one s and three p orbitals to form four equivalents sp^3 hybrid orbitals of the same energy and shape is called sp^3 hybridization. For example, carbon atom is sp^3 hybridized in CH_4 molecule.

In methane (CH_4) molecule, carbon atom forms four identical bonds by using four equivalent hybrid orbitals. These orbitals are the result of sp^3 hybridization, one s and three p-orbitals of carbon are mixed to form four sp^3 hybrid orbitals. These sp^3 orbitals are similar in shape and energy and become oriented at an angle of 109.5°.

C (Ground state)= $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0$

C (Excited state)= $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$

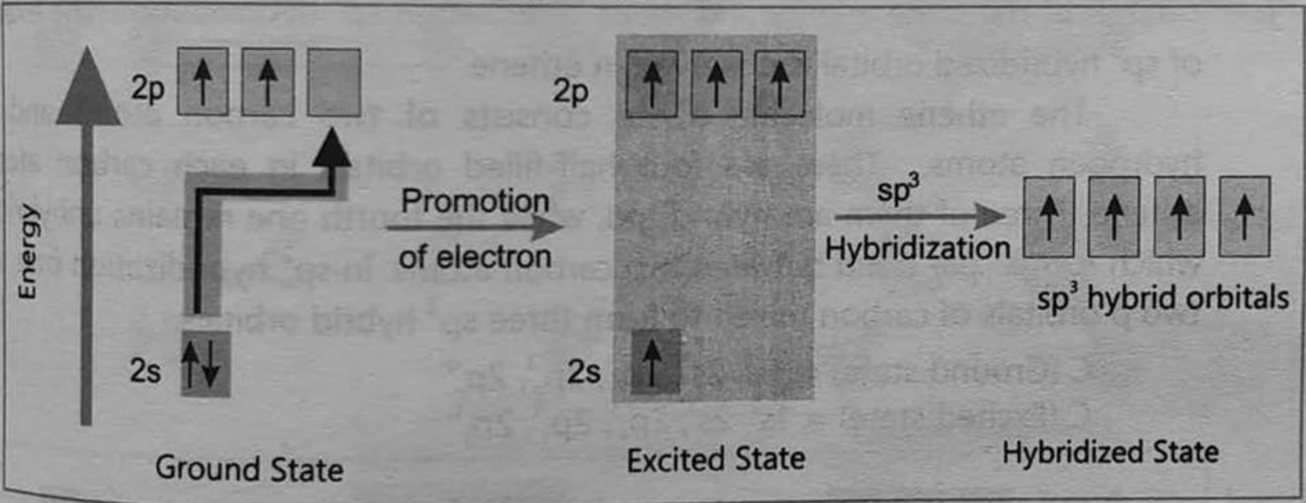


Figure 3.19 (a) sp^3 Hybridization

Each sp^3 hybrid orbital overlap with 1s orbital of hydrogen atom to form four C – H bonds. Thus, each hybrid orbital is composed of 25% s and 75% p character.

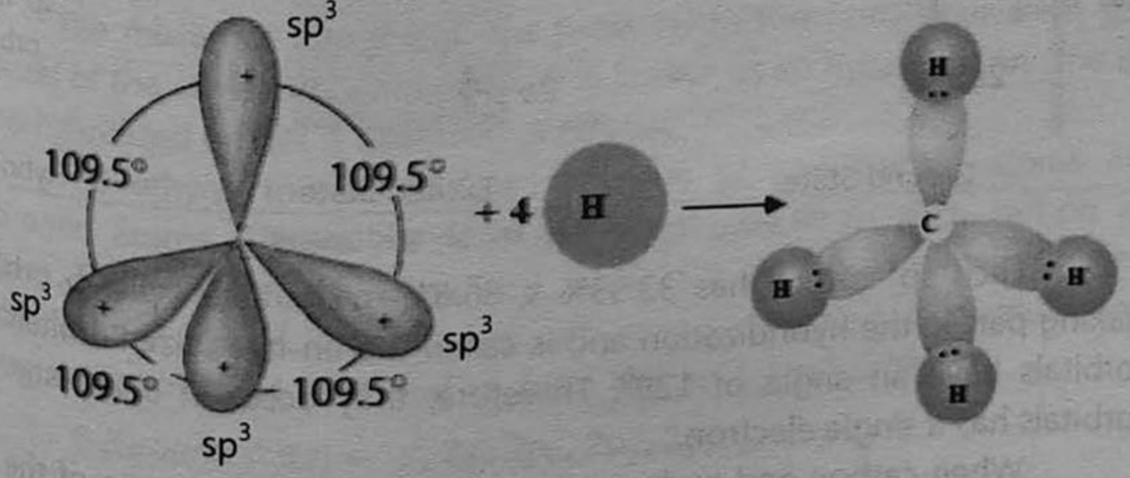
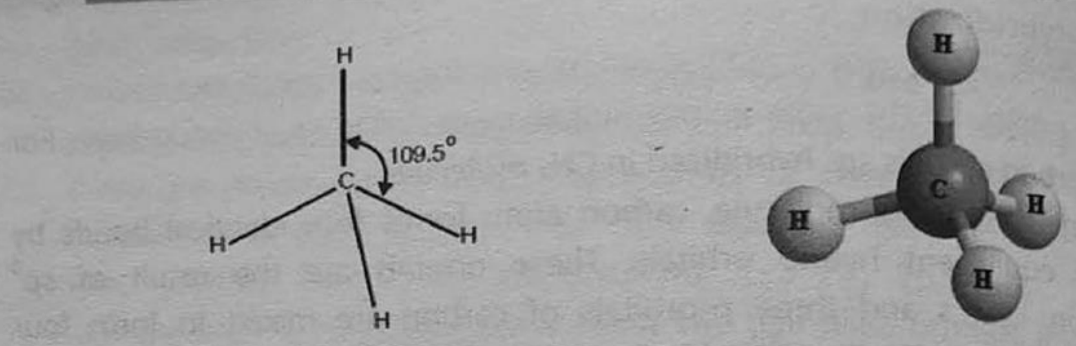


Figure 3.19 (b) sp^3 Hybrid Orbitals and Hydrogen Atoms



CH_4 Moleucle

Figure 3.20 Tetrahedral CH_4 Molecule

ii. sp^2 hybridization

The mixing of one s and two p-orbitals to form three equivalent sp^2 hy orbitals of the same energy and shape is known as sp^2 hybridization. The exa of sp^2 hybridized orbital is observed in ethene.

The ethene molecule (C_2H_4) consists of two carbon atoms and hydrogen atoms. There are four half-filled orbitals in each carbon ato ethene. Three of them are hybridized, while the fourth one remains unhybridi which forms pi– bond between two carbon atoms. In sp^2 hybridization one s two p orbitals of carbon mixed to form three sp^2 hybrid orbitals.

C (Ground state) = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0$
C (Excited state) = $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$

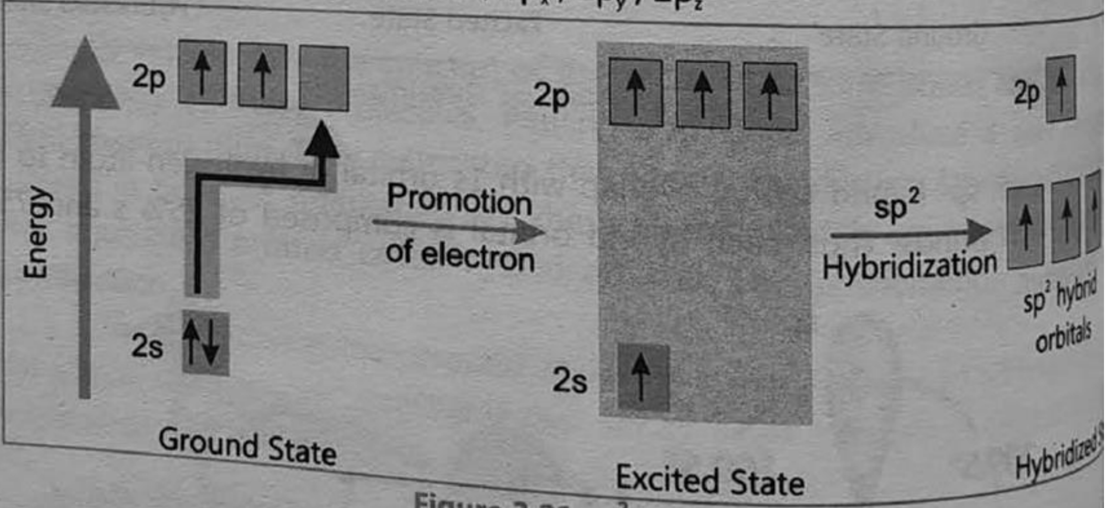


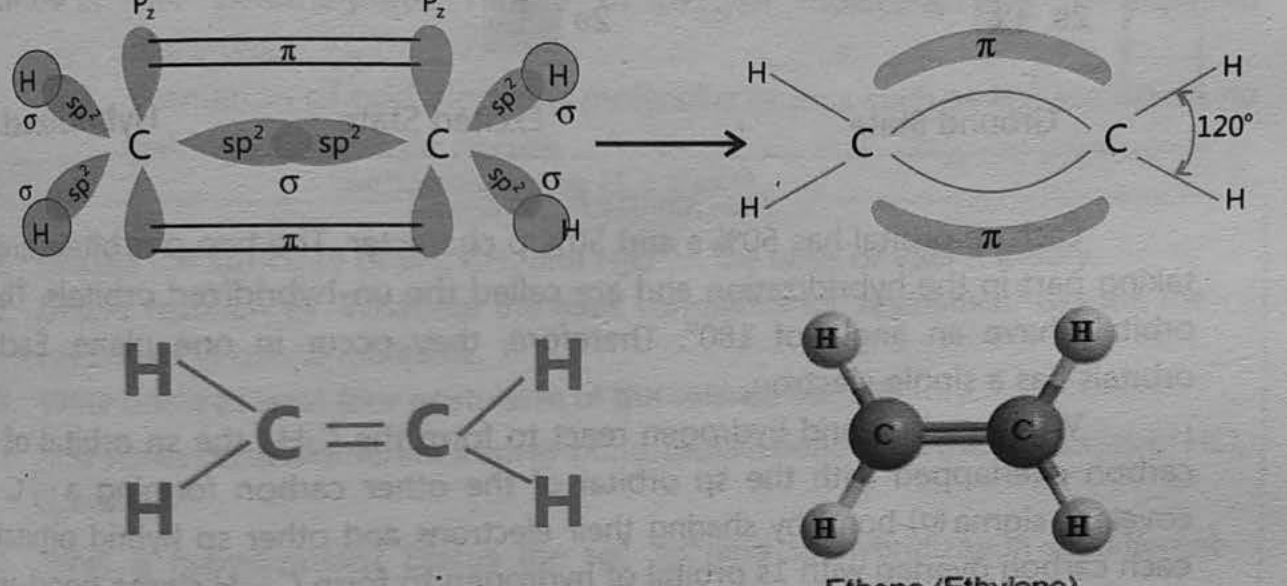
Figure 3.21 sp^2 Hybridization

Each sp^2 orbital has 33.33% s, 66.67 % p character. One p orbital is taking part in the hybridization and is called the un-hybridized orbitals. These orbitals have an angle of 120°. Therefore, they occur in one plane. Each orbitals has a single electron.

When carbon and hydrogen react to form the C_2H_4, one of the three orbitals of one carbon overlaps with sp^2 orbital of the other carbon, forming a C – C, covalent sigma (σ) bond by sharing their unpaired electron.

The remaining two sp^2 orbitals of each carbon overlap with two s orbitals of the two hydrogen atoms forming two more covalent (C – H) sigma bonds by the sharing of their unpaired electron.

As each carbon has one p un-hybridized, these orbitals also overlap sidewise with each other forming a weaker covalent bond called pi(π) bond.



Ethene (Ethylene)

Figure 3.22 Ethene Molecule

The double bond consists of one sigma and one π - bond. The bond length of C=C double bond is 1.34Å . The C – H bond length is 1.10Å. The bond angle is 120°. Thus, the structure of ethene is planer. There are five sigma bonds and one π - bond in ethene molecule.

iii. sp Hybridization

The mixing of one s and one p orbital to form two equivalent sp hybrid orbitals of the same energy and shape is known as sp hybridization. The example of sp hybridized orbital is observed in ethyne.

The ethyne molecule (C_2H_2) consists of two carbon atoms and two hydrogen atoms. There are four half-filled orbitals in each carbon atom in ethyne. Two of them are hybridized, while the other two remain unhybridized, which form pi – bond between two carbon atoms. In sp hybridization one s and one p orbitals of carbon mixed to form two sp hybrid orbitals.

C (Ground state) = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0$

C (Excited state) = $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$

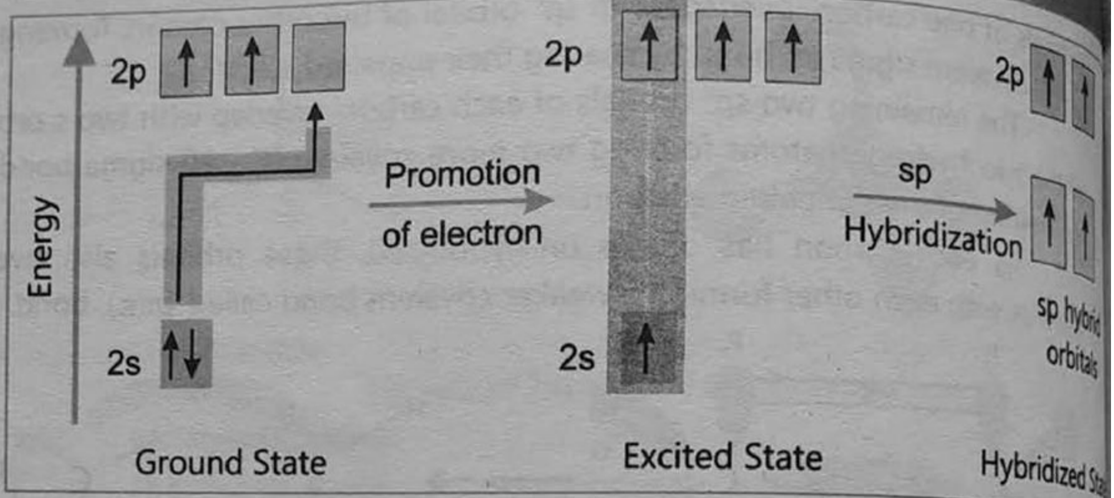


Figure 3.23 sp Hybridization

Each sp orbital has 50% s and 50% p character. The two p orbitals are no taking part in the hybridization and are called the un-hybridized orbitals. The s orbitals have an angle of 180°. Therefore, they occur in one plane. Each s orbitals has a single electron.

When carbon and hydrogen react to form the C_2H_2, the sp orbital of on carbon overlapped with the sp orbital of the other carbon forming a C - covalent sigma (σ) bond by sharing their electrons and other sp hybrid orbitals o each carbon overlap with 1s orbital of hydrogen to form C – H sigma bond, whi the two unhybridized p orbitals overlap sidewise to form two pi (π) bonds.

As each carbon has two un-hybridized p orbitals, which are bi-lobe dumbbell shaped. Their one lobe is above the plane and other lobe is below These orbitals also overlap with each other parallel or laterally forming pi-bond

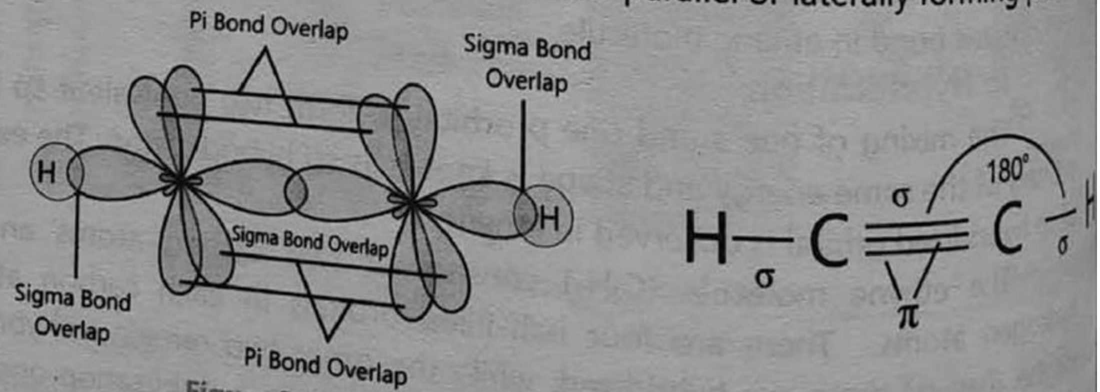


Figure 3.24 Overlapping of Orbitals and Ethyne Molecule

The ethyne (acetylene) molecules consists of triple bond between carbo atoms (C≡C) i.e. one sigma and two pi-bonds having a length of 1.20Å. The C –H bond length is 1.09Å . The bond angle is 180° and the shape o molecule is linear. Overall, there are three sigma and two pi-bonds (π – bonds) in the molecule of acetylene.

Shortcoming of Valence Bond Theory

Though the valence bond theory explains the bonding and geometry of many molecules and ions, but it failed to explain the,

1. Formation of coordinate covalent bond.
2. The paramagnetic nature of oxygen molecule, due to unpaired electrons.
3. Formation of odd electrons molecules or ions such as H_2^+ ion where no pairing of electrons occurs.

Self-Assessment

1. Discuss the structure of BF_3, CH_4 and H_2O on the basis of VSEPR theory.
2. Define resonance? What are the basic conditions for resonance? Discuss the resonance in ozone molecule.
3. Write down at least four postulates of the valence bond theory.
4. How sigma bond is different from pi-bond. Explain bonding in the molecules of HCl, Cl_2 and O_2.
5. What is hybridization? Discus the sp^3, sp^2 and sp hybridization in different molecules in detail.
6. What are the shortcomings of VBT?

STS Science, Technology and Society

Hair is composed of keratin, a strong fibrous protein. The hydrogen bonds and disulfide bonds are responsible for straight and curly hairs.

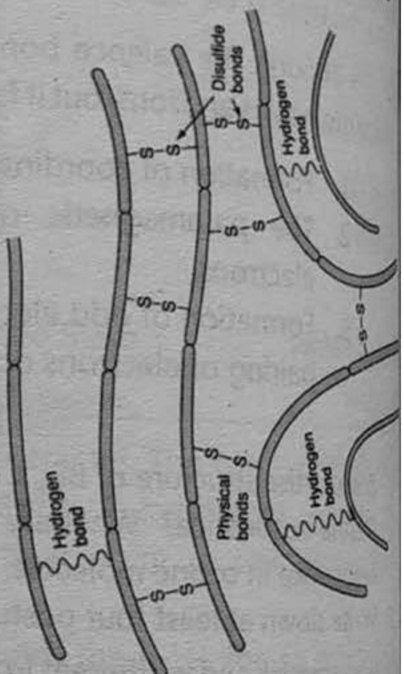
Hydrogen bonds

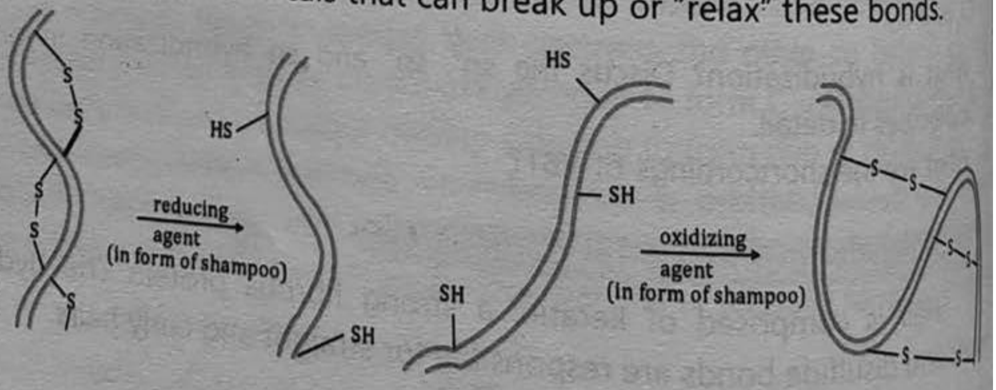
These bonds are the most flexible. Hydrogen bonds are easily broken in the presence of water and heat. They are the primary bonds responsible for changing our hair's overall shape. Hydrogen bonding allows our hair to change shape temporarily and produces a strong hold. When the hair is wet by either shampooing/conditioning or in the presence of humidity, the molecules enter the fibers, break up the hair's preset hydrogen bonds, and form new bonds. For example, hair is usually set in rollers while wet. The hair is then held in position until it dries. As the hair dries, hydrogen re-bonding occurs, but in the new "shape".

The hair will remain in the new "shape" until it is wetted with wate again and that can occur either through shampooing/conditioning or throug humidity.

Disulphide bonds

Disulphide bonds are also known as Cysteine bond, Sulphur bond or S-bond. There is a formation of α covalent bond called a disulphide bridge between the sulphur atoms on two cysteins on separate chains of keratin. These bonds are stronger than hydrogen bond. The more disulphide that occurs in the fiber, the curlier and kinkier the hair. These bonds cannot be broken by water or heat treatment. Only chemical agents can break these bonds. Therefore, if a person with curly hair wants straight hair, he/she would need to use chemicals that can break up or "relax" these bonds.





3.2.2 Molecular Orbital Theory (MOT)

In 1932, Hund and Mulliken put forward the molecular orbital theory. T theory explains the formation of covalent bond and paramagnetic properties molecules in a better way. According to molecular orbital theory, all atomic orbi of the atoms take part in the formation of molecule. Mix with one another to give to an equal number of new orbitals called molecular orbitals. The molecular orbi with lower energy are called bonding molecular orbitals and denoted by σ or π. T other with higher energy are called anti-bonding molecular orbitals denoted by σ π*. The main features of molecular orbital theory are as under.

1. All the molecular orbitals have definite energy. Their relative energies are,
   $\sigma 1s < \sigma^*1s < \sigma 2s < \sigma^*2s < \sigma 2p_x < \pi 2p_y = \pi 2p_z < \pi^* 2p_y = \pi^* 2p_z < \sigma^* 2p_x$
2. The arrangement of electrons in molecular orbitals occurs according to the Pauli's exclusion principle, Aufbau principle and Hund's rule.
3. The sigma (σ) and pi (π) notation are used in the same way as they are used in the valence bond theory but here the bonding molecular orbital (B.M.O) are σ and π, while the anti-bonding molecular orbitals (A.B.M.O) are σ* and π*.

The number of bonds in a molecule is one-half of the difference of the number of electrons in the bonding molecular orbital and the number of electrons in the anti-bonding molecular orbitals and is called bond order.

Mathematically,

$$\text{Bond order} = \frac{\left(\begin{array}{c}\text{No.of electrons in}\\ \text{bonding molecular orbitals}\end{array}\right) - \left(\begin{array}{c}\text{No. of electrons in}\\ \text{anti-bonding molecular orbitals}\end{array}\right)}{2}$$

Usually in practice, only molecular orbitals formed from the valence orbitals are considered for determining bond order.

ReadingCheck

Define bond order.

Applications of Molecular Orbital Theory

i. Hydrogen Molecule (H_2)

The atomic number of hydrogen is one. Its electronic configuration is '$1s^1$'. Hydrogen molecule (H_2) is formed by the overlap of two $1s^1$ atomic orbitals of two hydrogen atoms. They produce two molecular orbitals. One is bonding molecular orbital (B.M.O) σ(1s) and the other is anti-bonding molecular orbitals (A.B.M.O) σ*(1s). The molecule has two electrons to be filled in these molecular orbitals. According to Aufbau principle both these electrons will enter in the lower energy bonding molecular orbitals (B.M.O) and the anti-bonding molecular orbitals (A.B.M.O) remains vacant. The electronic configuration of the molecule is represented by the equation:

$$2H\,(1s^1) \longrightarrow H_2\,[\sigma(1s^2)\,\sigma^*(1s^0)]$$

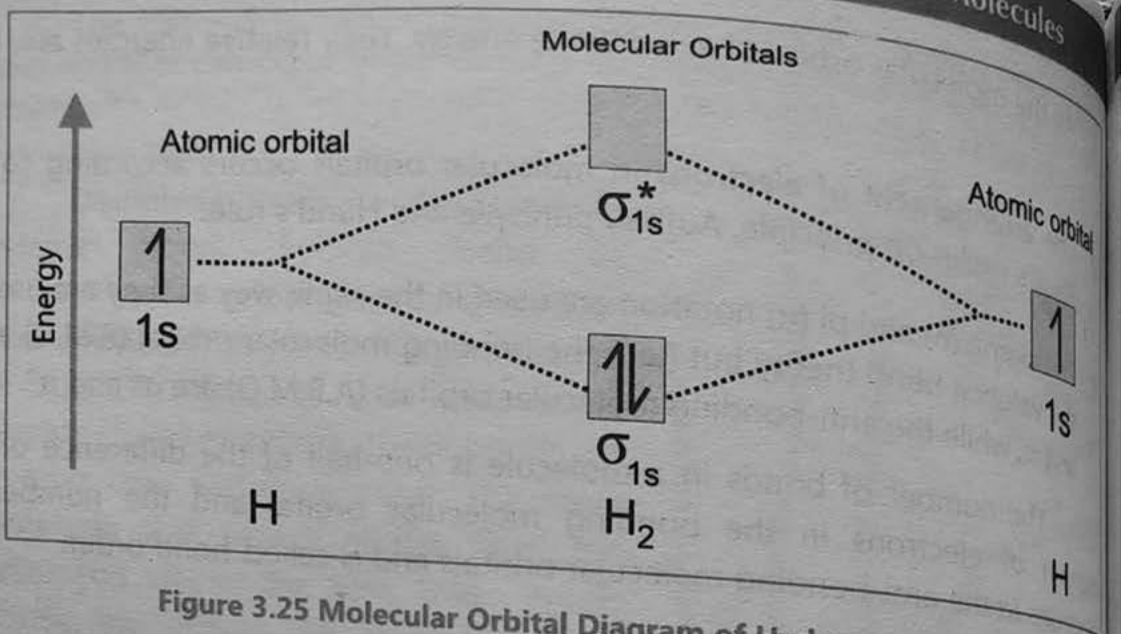


Figure 3.25 Molecular Orbital Diagram of Hydrogen Molecule

The number of bonds in the molecule is,

$$\text{Bond order} = \frac{(\text{No. of electrons in BMO's}) - (\text{No. of electrons in ABMO's})}{2}$$

$$\text{Bond order} = \frac{(2-0)}{2} = \frac{2}{2} = 1$$

Thus, the two hydrogen atoms are bonded through only one bond in th molecule.

ii. Helium Molecule (He_2)

The atomic number of 'He' is two. Its electronic configuration is Is^2. Tw atomic orbitals of two He atoms combine to produce two molecular orbitals. One bonding molecular orbital (B.M.O) σ(1s) and the other is anti-bonding molecu orbitals, (A.B.M.O) σ* (1s). The molecule has four electrons to be filled in the molecular orbitals. According to Aufbau principle two electrons enter in the low energy bonding molecular orbitals (B.M.O) σ(1s) and the other two electrons en the anti-bonding orbitals (A.B.M.O) σ*(1s). The electronic configuration of th molecule is represented by the equation:

$$2He\ (1s^2) \longrightarrow He_2\ [\sigma\ (1s^2)\ \sigma^*(1s^2)]$$

Each one of these molecular orbitals would accommodate two elec as shown in the figure 3.26.

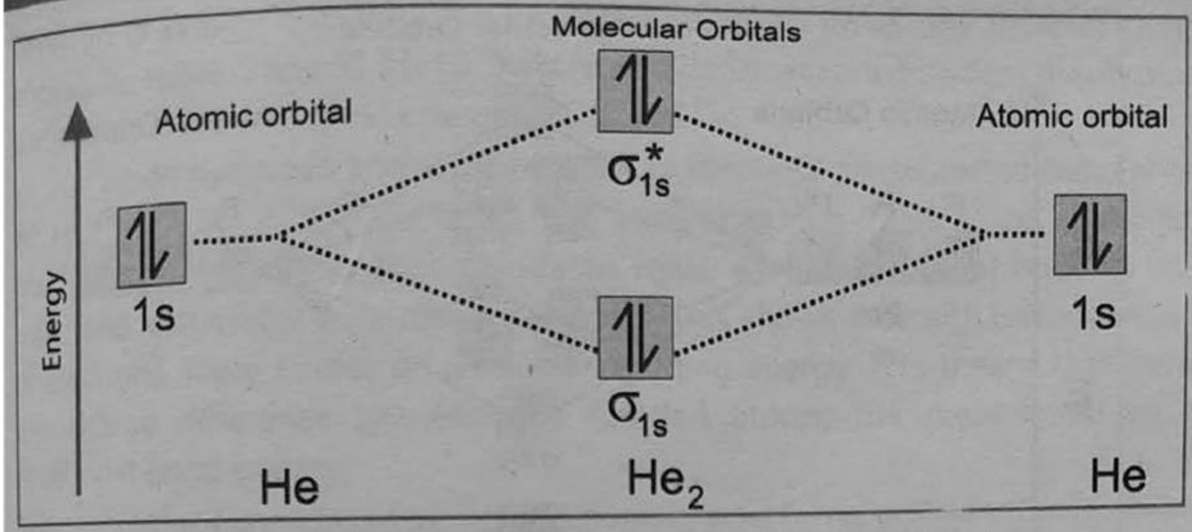


Figure 3.26 Molecular Orbital Diagram of Helium Molecule

The number of bonds in the molecule is,

$$\text{Bond order}=\frac{(\text{No.of electrons in BMO's})-(\text{No.of electrons in ABMO's})}{2}$$

$$\text{Bond order} = \frac{(2-2)}{2}=0$$

As bond order is zero so no bond is formed in He_2. It means that this molecule does not exist.

iii. Oxygen Molecule (O_2)

The atomic number of Oxygen is eight. Its electronic configuration is $1s^2$, $2s^2$, $2p_x^2, 2p_y^1, 2p_z^1$. Each oxygen atom contributes six electrons to O_2 molecule from its valence shell. The two participating oxygen atoms contribute a total of $2(2+2+1+1) = 12$ valence electrons, There are eight molecular orbitals and 12 electrons are accommodated in them as shown in Fig. 3.29.

The molecule of oxygen is represented by the equation.

$$2O(1s^2, 2s^2, 2p_x^2, 2p_y^1, 2p^1{}_z) \longrightarrow O_2[\sigma(2s^2), \sigma^*(2s^2), \sigma 2p_x^2, \pi 2p_y^2 = \pi 2p_z^2, \pi^* 2p_y^1 = \pi^* 2p_z^1, \pi^* 2p_x^0]$$

The electronic configuration of the molecular orbitals and presence of the two unpaired electrons is responsible for the paramagnetic behaviour of oxygen molecule. The unpaired electrons create a magnetic field around them due to their spin.

The explanation of paramagnetic behaviour of O_2 molecule is the greatest success of the Molecular Orbital Theory. Both VSEPR theory and VBT fail to explain the paramagnetic property of oxygen molecule.

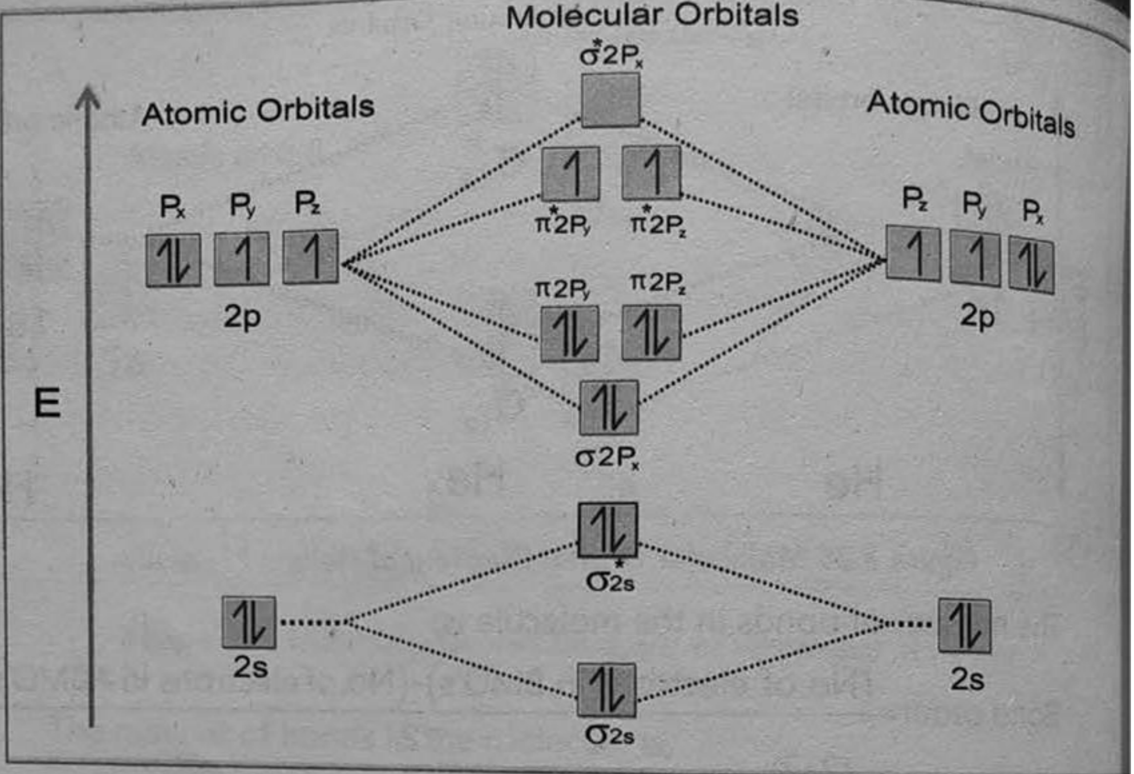


Figure 3.27 Molecular Orbitals Diagram of Oxygen Molecule

The number of bonds in the molecule is,

$$\text{Bond order}=\frac{(\text{No. of electrons in BMO's})-(\text{No. of electrons in ABMO's})}{2}$$

$$\text{Bond order} = \frac{(8-4)}{2}=\frac{4}{2}=2$$

There are two bonds in the oxygen molecule.

3.3 Bond Characteristics

3.3.1 Bond Energy

Bond energy is defined as *the amount of energy required to break mole of bonds in gaseous substance to form neutral atoms (also in gas state).*

Thus, bond energy is the measure of the strength of a bond: the large bond energy, the stronger the chemical bond and vice versa. It depends u electro-negativity, size of the atoms and bond length. The S.I unit of bond ene is $kJ.mol^{-1}$.

The energy required to break one mole of hydrogen molecule $436 kJ.mol^{-1}$ and 72.42×10^{-23}kJ is required to break one bond. The sharing electrons between the two bonded hydrogen atoms is equal, so each bo hydrogen atom contributes 36.21×10^{-23}kJ energy per atom, which is half of total bond energy. Similarly, the energy required to break one mole of chlorine molecules is 243kJ and 40.34×10^{-23}kJ is required to break one bond or contribution of each Cl atom towards bond energy is 20.17×10^{-23}kJ.

When hydrogen and chlorine react to form HCl the expected bond energy of HCl is 56.38×10^{-23}kJ / bond but experimentally 72.39×10^{-23}kJ/bond is produced. This is higher than calculated value, which shows that bond in HCl is polar and is stronger than non-polar bond. This shows that with unequal sharing of electrons, there comes an additional binding energy. This means that greater the charge difference between the bonded atoms, the greater will be the additional bond energy.

Table 3.2 Comparison of Experimental and Calculated Bond Energy of Hetero Nuclear Molecules

Bond	*Bond energies* $(KJ\,mole^{-1})$			
	$X=F$	$X=C\ell$	$X=Br$	$X=I$
H–X (calculated)	293	236	311	291
H–X (experimental)	567	436	366	299
Difference	274	200	55	9

The bond energies of carbon to carbon being in order of C≡C>C=C>C–C, the bond length is in reverse order C–C>C=C>C≡C. The bonds with higher bond energy values have shorter bond length.

3.3.2 Bond Length

Bond length is defined as the mean distance between the nuclei of two covalently bonded atoms in a molecule. Bond lengths are determined experimentally using X-ray diffraction or the analysis of molecular spectra. The length of a chemical bond is the result of an equilibrium between attractive and repulsive forces of the bonded atoms.

The bond length is measured in angstrom (Å), nanometer (nm) or picometer (pm). The bond length of identical diatomic molecules having identical atoms is the sum of the radii of these atoms. For example, the bond length of the C – C is 154pm and bond length of Cl – Cl is 198pm.

For hetero-nuclear diatomic molecules, bond length become shortened and deviates from the calculated sum of individual covalent radii, due to increase in difference of electronegativity. For example, experimentally calculated bond length of HCl is 127pm, whereas the calculated value for atomic radii of H= 37pm and Cl = 99pm gives H – Cl bond length equals to 136pm. The calculated values are always higher than experimental values for heteronuclear molecules. This is due to the difference in electronegativity, which produces polarity. This result in shortening of bond length due to the force of attraction between the polar ends. This can easily be observed in table 3.2.

Table 3.3 Comparison of Experimental and Calculated Bond Lengths of Heteronuclear Molecu

Bond	Bond length in pm(picometer)		
	Calculated value	Experimental value	Difference
H – F	108	92	16
H – Cl	136	127	09
H – Br	151	141	10
H – I	171	161	10

3.3.3 Ionic Character

The type of bond between any two atoms in a molecule can b determined from the difference of electronegativities values of the two bonde atoms. A molecule composed of two identical atoms, its electronegativ difference is zero, and hence is always non-polar and does not have any ioni character.

On other hand, when a molecule is formed between two different atom that have different electronegativity values, such a bond is polar in nature an has an ionic character. If the difference of electronegativity between two bonde atoms is less than 0.4, it is non-polar bond. If the difference of electronegativity i from 0.4 – 1.7, bond will be polar with some ionic character. If the difference o electronegativity is greater than 1.7, the bond will be ionic in character.

3.3.4 Dipole Moment

A quantitative measure of the polarity of a bond is its dipole moment (which is the product of the charges 'q' and the distance 'r' between the centres o charges.

Mathematically it can be expressed as,

$$\mu = q \times r \qquad (3.1)$$

Where 'q' is charge and 'r' is distance between centres of charges. T direction of the dipole is shown by the sign $+\!\!\!\longrightarrow$ .The arrow points to the parti negatively charged end of the dipole. For example,

$$\overset{+\delta}{H} \; \underline{\xrightarrow{\mu}} \; \overset{-\delta}{Cl}$$

For complicated molecules, the net dipole moment is the vector sum of the individual bond moments. To keep the molecule electrically neutral, t charges on both ends of the diatomic molecule must be equal in magnitude a opposite in sign. However, in equation (3.1), 'q' refers only to the magnitude the charge and not to its sign, so 'μ' is always positive.

Dipole moments are usually expressed in Debye units (D). In SI syste charges are expressed in Coulombs (C) and distance in meters (m); thus, dipole moment is expressed in unit of coulomb meter (Cm) in SI system. The conversion factor is

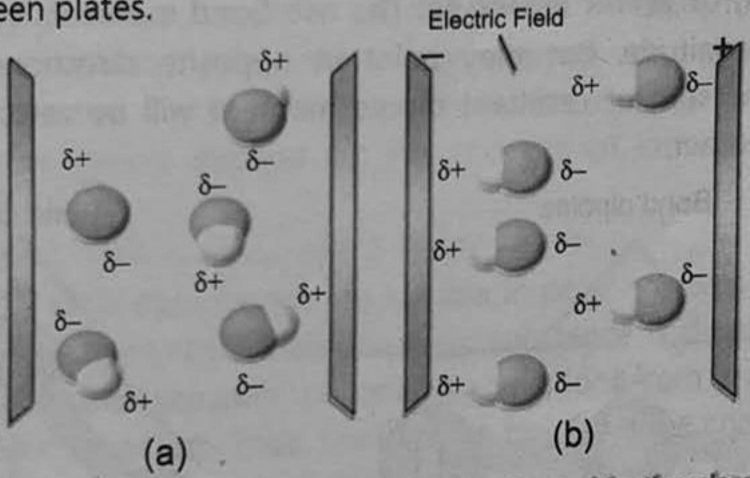
$$1\ \text{D} = 3.336 \times 10^{-30}\ \text{Cm}$$

Measurement of Dipole Moment

The dipole moment of a substance can be experimentally measured with the help of an electric condenser. When condenser is charged by connecting to battery, electric field is set up with field strength equal to the applied voltage divided by distance between plates.

ReadingCheck

1. What is bond energy?
2. What is dipole moment?



(a) (b)

Figure 3.28 (a) Molecules are always randomly distributed in the absence of an electric field. (b) When an electric field is applied, polar molecules like HF will align to the dipoles with the field direction

When polar molecules are placed between charged plates these molecules, align themselves with negative end toward positive plate and positive end toward negative plate. As a result, a decrease in strength of electric field is observed. From this decrease in strength of electric field, the dipole moment is determined.

Application of Dipole Moment

Dipole moment provides two types of information about the molecule's structure.

a. Percentage of ionic character of bond

From experimentally determined dipole moments, the percentage of ionic character of bond can be calculated by the following formula.

$$\text{Percentage of ionic character} = \frac{\mu_{\text{observed}}}{\mu_{\text{ionic}}} \times 100$$

μ_{observed} is experimental value of dipole moment of the molecule and

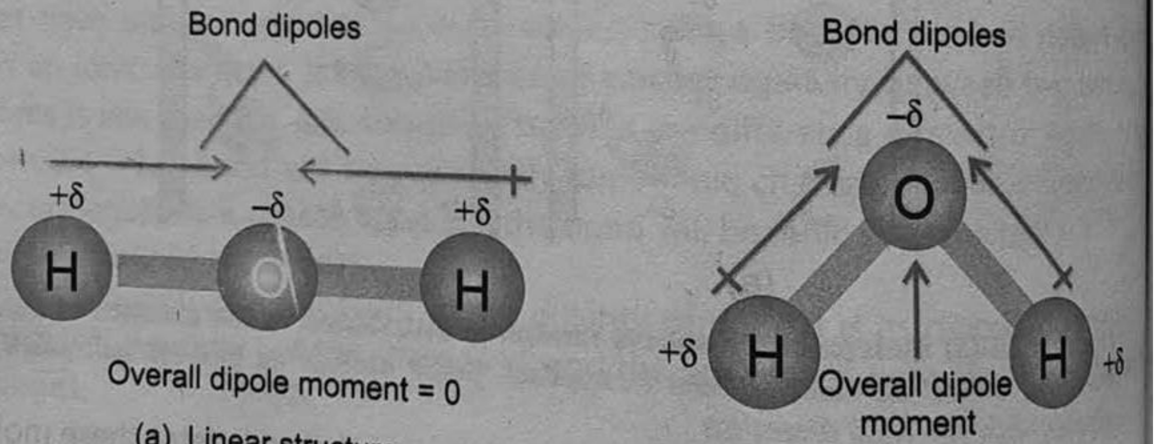
μ_{ionic} is dipole moment of molecule if it is 100% ionic. Greater the percent ionic character of a molecule higher will be its polarity.

b. Determining the Geometry of the Molecule

Dipole moment can provide important information about the geometry of the molecules. If two or more geometrical shapes for a molecule are possible then the correct structure can be identified from the study of its dipole moment. For example, Water has two possible structures, linear and angular as shown in figure 3.28.

The arrows show the shift of electron density from the less electronegative hydrogen atoms to the more electronegative oxygen atom.

Structure (a) of Water Molecule: The two bond moments of O – H bonds are equal in magnitude. But they point in opposite directions in a linear H_2O molecule, the sum or resultant dipole moment will be zero, because they will cancel each other.



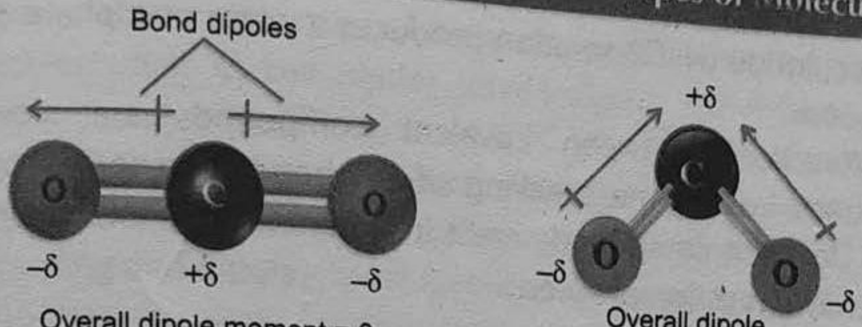
(a) Linear structure

(b) Angular structure

Figure 3.29 Bond Dipoles in Water Molecule

Structure (b) of Water Molecule: On the other hand, if the H_2O molecule was bent, the two bond moments would partially reinforce each other, so that the molecule would have a dipole moment. Experimentally it is found that water has 1.84D dipole moment. Therefore, we conclude that the water molecule has angular shape 3.31(b) and not a linear 3.31(a).

Carbon dioxide (CO_2) does not have any dipole moment as shown in figure 3.32(a). The reason is that CO_2 has linear structure. It has two polar C=O bonds acting in opposite directions. They cancel out the effect of each other, so the molecule as a whole is non-polar. *If the bonds dipoles in a molecule do not cancel out each other exactly, the molecule is polar.*



Overall dipole moment = 0
(a) Linear structure

Overall dipole moment
(b) Bent structure

Figure 3.30 Bond Dipoles in Carbon dioxide (CO_2) molecules

3.4 Effect of Bonding on Physical and Chemical Properties

The type of bonding present in substances characterizes the properties in them. Physical properties of compounds depend on the strength of intermolecular attractive forces (Van der Waals forces). On the other hand, chemical properties mainly depend on the strength of intra-molecular forces (bond strength).

3.4.1 Solubility of Ionic and Covalent Compounds

Most of the ionic compounds are soluble in polar solvents like water but insoluble in non-polar solvents. When an ionic substance is dissolved in water, the polar water molecules separate the cations and anions from the crystal lattice by their electrostatic attraction. Thus, the ions are free from the crystal lattice and ionic compound dissolve in water. Non-polar solvents, like Benzene, do not dissolve ionic compounds because the attraction between solvent and solute molecules is negligible.

A Non-polar compound (solute) dissolves in a non-polar solvents. This is due to presence of weak Van der Waals forces are present in it. These weak attractive forces of solvent overcome attractive forces among solute molecules. From the above discussion, you can conclude that **"Like Dissolves Like"**.

3.4.2 Reactions of ionic and Covalent Compounds

Ionic compounds usually do not react in solid state because the ions are very tightly held together. When they are dissolved in water, the oppositely charged ions separate from one another and become ready for a chemical reaction.

When aqueous solutions of two ionic compounds are mixed together, very rapid reaction takes place and new product is formed. This is because, as there is no bond breaking is involved in solutions, on mixing solutions, ions combined and new bonds are formed, for example, mixing of silver nitrate ($AgNO_3$) and sodium chloride (NaCl) solution produces a white precipitate of silver chlori milliseconds.

Reactions between covalent compounds are slow because th compounds involve the breaking of old bonds and formation of new cova bonds. Covalent compounds react in different ways and their reaction depe on the way a reaction proceeds.

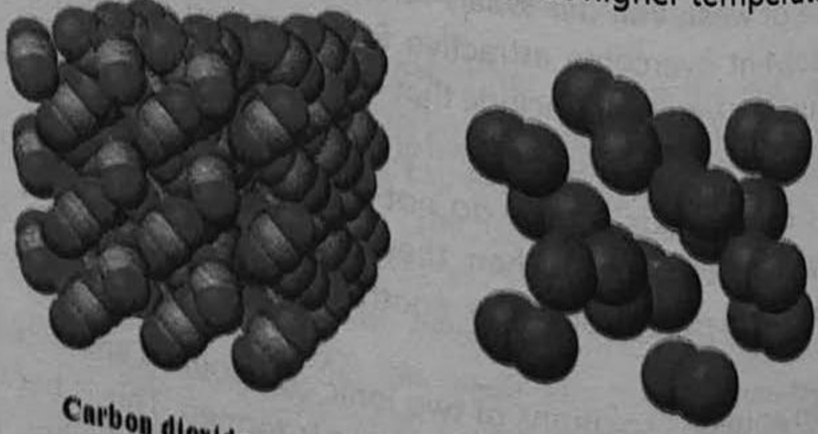
3.4.3 Directional and Non-Directional Nature of Ionic and Cova Compounds

There is a marked difference between ionic and covalent bonds. Ionic bo are non-directional whereas covalent bonds are directional in nature. That is why t covalent molecules have definite geometry. This is due to the fact covalent bo are formed by overlapping of atomic orbitals, which have definite direction. Dur covalent bond formation, these atomic orbitals overlap each other when they ar proper direction. This gives definite geometric shape to the atoms in molecules. T covalent bonds are directional, for example, the covalent bond in methane (CH directional in nature. The four sp^3 hybridized orbitals of carbon make an angle 109.5° with each other. The hydrogen atom can only make bond with these orbita they approach at angle 109.5° to carbon atom.

3.4.4 Molecular, Network and Metallic Solid

a. Molecular Solids

Molecular solids are, made up of molecules. Like atomic solids, t molecules that make up molecular solids, such as ice, sugar and iodine a composed of neutral molecules. Substances consisting of larger, nonp molecules have larger attractive forces and melt at higher temperatures.



Carbon dioxide

Iodine

Figure 3.31 Molecular Solids of Carbon dioxide (CO_2) and Iodine (I_2)

Molecular solids composed of molecules with permanent dipole moments (polar molecules) melt at still higher temperatures. For example, the melting point of non-polar propane (C_3H_8) is −190°C. A molecule of polar formic acid (HCOOH), which has a similar number of electrons and the same molar mass as propane, melts at 8.4°C. The large difference in boiling point is due to the hydrogen bonding and dipole-dipole forces in formic acid.

b. Network Solids (Macro Molecules)

Unlike the intramolecular covalent bonds that hold atoms together in separate molecules, it is possible for atoms to bond covalently into continuous two or three-dimensional arrays, called *network solids*. A wide range of properties can be found among network solids. Diamond and graphite are examples of network solids.

In diamond, each carbon atom forms single covalent bonds to four other carbon atoms, which are at the corners of a tetrahedron. The four carbon atoms are, in turn, covalently bonded to four other carbon atoms and so on. This bonding exists throughout the entire crystal. When all the atoms in a crystal are covalently bonded to one another throughout the whole crystal, the solids are termed network solids.

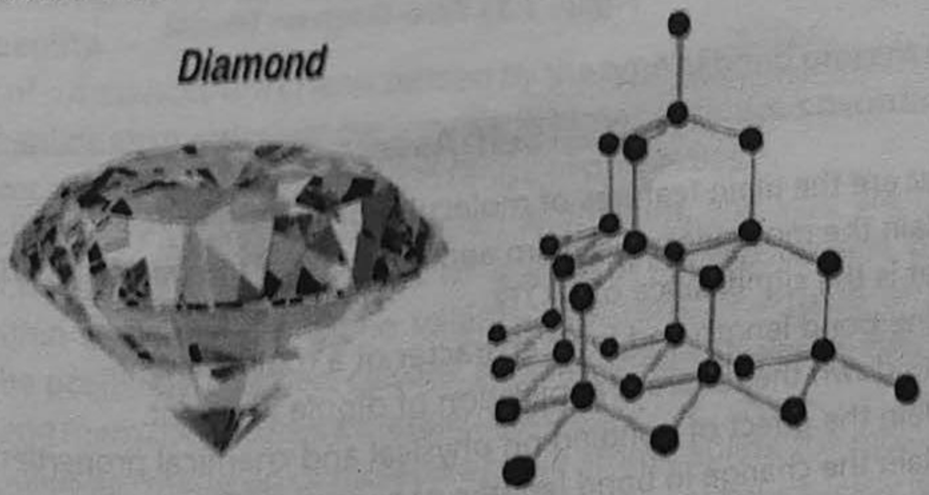


Figure 3.32 Diamond

c. Metallic Solids

Metallic solids such as crystals of copper, aluminium and iron are formed by metal atoms. Metals are composed of a closely packed centers of metallic cations, within delocalized, mobile valence electrons. The force of attraction between the positively charged cations and the pool of valence electrons that moves among them constitutes a metallic bond.

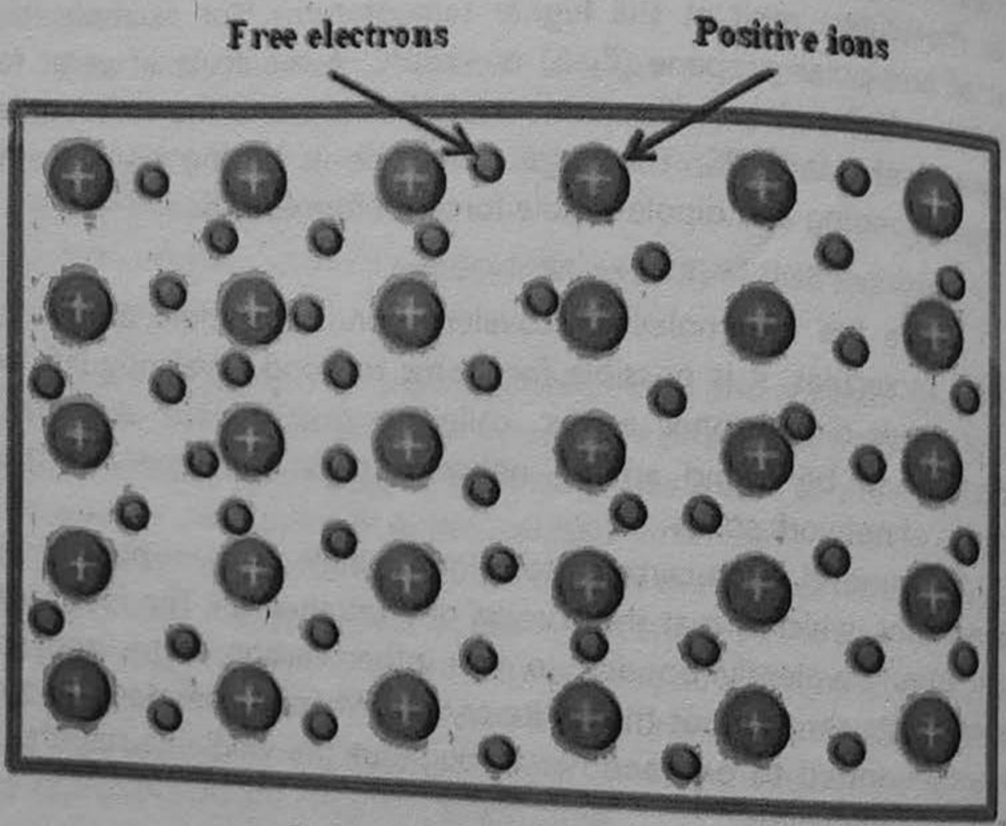


Figure 3.33 Free-Electron Model

Self-Assessment

1. What are the main features of molecular orbital theory?
2. Explain the molecules of Helium and Oxygen on the basis of MOT.
3. What is the significance of MOT?
4. Define bond length and ionic character of a molecule.
5. Write down the different application of dipole moment.
6. Explain the effect of bonding on physical and chemical properties.
7. Explain the change in bond lengths of hetero-nuclear molecules due to difference in electronegativity values of bonded atoms.
8. Explain the difference between molecular, network and metallic solid.

KEY POINTS

- Chemical bonds are forces that hold the atoms together in molecules.
- Covalent bonds are formed by the sharing of electrons.
- VSEPR theory tries to explain the geometry of the molecules.
- Resonance structures are models that give the same relative position of atoms as in Lewis structures but show different places for their bonding and lone pairs.
- In valance bond theory (VBT), the overlapping of atomic orbitals form a covalent bond.
- In molecular orbital theory (MOT), combination of atomic orbitals forms molecular orbitals.
- The intermixing of different atomic orbitals to form equivalent orbital called hybrid orbital is known as hybridization.
- Bond energy is the energy required to break the bonds per mole to form individual atoms.
- Bond length is the mean distance between the nuclei of the two bonded atoms.
- Dipole moment (μ) is a product of charge and distance between the charges. It is a vector quantity.
- Properties of substances are characterized by the type of bond present in them.
- In Network solids atoms are bonded covalently into continuous two-dimensional or three dimensional arrays with a wide range of properties.
- Metallic solids such as crystals of copper, aluminium, and iron are formed by metal atoms. Metals are composed of a closely packed centers of metallic cations, within delocalized, mobile valence electrons. The force of attraction between the positively charged cations and the pool of valence electrons that moves among them constitutes a metallic bond.
- Molecular solids are made up of molecules. Like atomic solids, the molecules that make up molecular solids, such as ice, sugar and iodine are electrically neutral.

EXEERCISE

Choose the correct option.

1. The head on overlap of p–orbitals of two atoms give rise to bond called,
   - a. Sigma bond
   - b. Pi (π) bond
   - c. Ionic bond
   - d. Metallic bond
2. Which one of the following molecules has a pyramidal structure?
   - a. CH_4
   - b. NH_3
   - c. H_2O
   - d. C_2H_4
3. Specie in which the central atom uses sp^2 hybrid orbitals in its bonding is,
   - a. PH_3
   - b. NH_3
   - c. CH_3^+
   - d. SbH_3,
4. On the basis of VSEPR theory, a molecule with three bond pair and no lone pair of electrons will have a structure
   - a. Linear
   - b. Trigonal planar
   - c. Tetrahedral
   - d. Trigonal pyramidal
5. Which of the following is an example of a network solid?
   - a. Sugar, $C_{12}H_{22}O_{11(s)}$
   - b. Graphite , $C_{(s)}$
   - c. Carbon dioxide, $CO_{2(s)}$
   - d. Magnesium fluoride, $MgF_{2(s)}$
6. All are true for π-bond except
   - a. π-bond is formed from sp hybrid orbitals
   - b. π-bond is formed by the parallel overlap of half filled p–orbitals
   - c. π-bond is formed when a sigma bond is already present
   - d. π-bond is weaker than sigma bond
7. Which one of the following molecules has zero dipole moment
   - a. NH_3
   - b. NF_3
   - c. BF_3
   - d. H_2O
8. The bond angle in H_2O is
   - a. 90°
   - b. 109.5°
   - c. 180°
   - d. 104.5°
9. Which one of the following compounds has the highest ionic character
   - a. HF
   - b. HCl
   - c. HBr
   - d. HI
10. Liquid oxygen is
    - a. Diamagnetic
    - b. Paramagnetic
    - c. Antimagnetic
    - d. Ferromagnetic

11. In Carbon dioxide (CO_2) molecule, the number of sigma covalent bond(s) is/are,
    a. 1   b. 2
    c. 3   d. 4
12. H_2S has a net dipole moment while BeF_2 has zero dipole moment, because
    a. H_2S molecule is linear while BeF_2 is angular
    b. H_2S molecule is angular, while BeF_2 molecule is linear
    c. Fluorine has more electronegativity than S
    d. Be is more electronegative than S
13. Which one has the least bond angle
    a. NH_3 b. H_2O
    c. CH_4 d. BF_3
14. The bond order in O_2 molecule is
    a. Zero   b. 1
    c. 2   d. 3
15. The unhybridized "p" orbital in sp^2 hybridization is
    a. parallel to sp^2
    b. in the same plane
    c. perpendicular to sp^2 orbitals
    d. out of plane

Short Questions

1. What evidence can you find that the CO_2 molecule has linear but H_2O molecule has angular structure?
2. Give the reason that why O_2 molecule is paramagnetic.
3. What ideas justify that the bond angle in NH_3 is 107.5° but in H_2O, it is 104.5°?
4. Differentiate between atomic and molecular orbitals.
5. What data was used to make the conclusion that the calculated bond lengths of the heteronuclear molecules are always higher than experimental values?
6. How would you prove that the sigma (σ)-bond is stronger than pi (π)-bond?
7. What information would you use to support the view that the molecule of the He_2 does not exist?
8. Differentiate between bonding and anti-bonding orbitals.

9. Give reason that why the structure of BF_3 is trigonal planar and NH_3 is trigon pyramidal.
10. Why the bond energies of polar molecules are higher than the non-pola molecules?

Descriptive Questions

1. (a) Draw a Lewis structure for $AlCl_3$, PH_3 and H_2O. Use VSEPR theory to predict the molecular shape of these molecules.
   (b) What VSEPR notations correspond to molecules that have a bent shape?
   (c) Discuss the different types of overlapping that lead to sigma bond formation.
2. (a) Explain how σ and π bonds are similar and how they are different.
   (b) Define and explain resonance with suitable example.
   (c) Discuss the (i) Bond energies (ii) Bond length and (iii) Ionic character with suitable examples.
3. (a) Explain the HCl, H_2O and N_2 molecules on the basis of valance bond theory.
   (b) Define and explain hybridization with reference to sp mode of hybridization.
   (c). Describe how knowledge of molecular polarity can be used to explain some physical and chemical properties of molecules?
4. (a) Write down the main points of molecular orbital theory.
   (b) Draw the bonding in the molecule of oxygen with the help of molecular orbital theory.
   (c) Explain with the help of MO theory, the paramagnetic character of oxygen.
5. (a) How the geometry of the molecule can be determined by using the dipole moment.
   (b) How could you measure the dipole moment of a molecule?
   (c) Write down the difference among molecular,network and metallic solids.

Project:

Use ball and stick models to represent the molecules of BF_3 and NH_3 in front of your class.