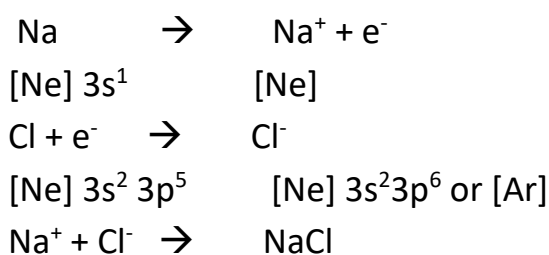


Example: Formation of NaCl –



- The electrostatic attraction between positive and negative ions leads to formation of bond which is known as electrovalent bond.

Octet Rule

- In 1916 Kossel and Lewis propounded the electronic theory of chemical bonding; which state that atom can combine by transfer of valence electrons from one atom to another or by sharing of valence electrons in order to complete the octet. This is called octet rule.

Covalent Bond

- In 1919 Langmuir introduced the term covalent bond.
- It can be explained by the formation of chlorine molecule.

Electronic configuration of Cl = $[\text{Ne}]3s^2 3p^5$

Here one electron is less in order to attain argon configuration. This purpose can be attained by formation of a sCl_2 molecule.

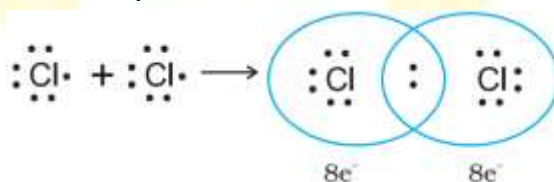
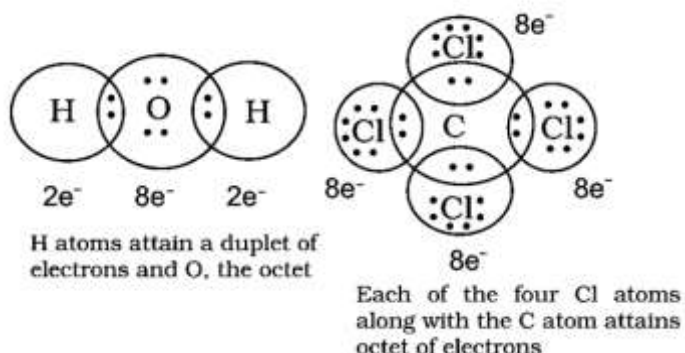


Figure: Covalent bond between two Cl atoms

- The electrons are represented by dots. Such structures are called Lewis dot structures.
- The important conditions to make Lewis dot structure-
 - a. Each bond is formed due to sharing of electron pair between the atoms.
 - b. Each combining atom contributes minimum one electron to the shared pair.

c. After the sharing of electrons, the combining atoms attain the outer shell noble gas electronic configuration.

d. Example:



- A single covalent bond formation takes place by sharing one electron pair between two atoms.
- When two atoms share two electron pairs the covalent bond is known as a double bond.

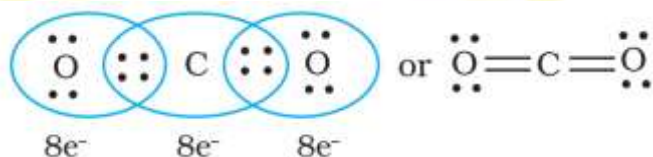


Figure: Double bond in CO₂ molecule

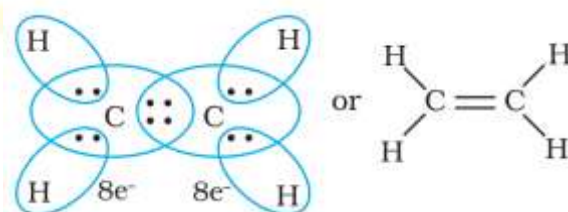


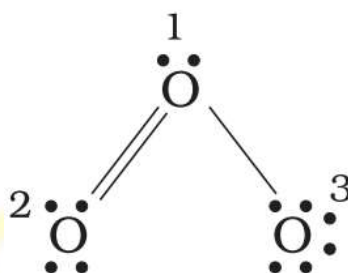
Figure: C₂H₄ molecule

- When three electron pairs are shared by combining atoms for example in N₂ molecule two nitrogen atoms and in ethyne molecule two carbon atoms make triple bond.

- The difference between the valence electrons of isolated atom and to number of electrons on that atom in the Lewis structure is known as formal charge.
- **Formal charge (F.C.) on an atom in a Lewis structure =**

[Total no. of valence electrons in the free atom] – [Total no. of nonbonding electrons] – $\frac{1}{2}$ [Total number of bonding electrons]

- For example: Ozone molecule (O_3)



- Here the atoms have been numbered as 1, 2, and 3.
- The formal charge on central O atom number 1:

$$= 6 - 2 - \frac{1}{2}(6) = +1$$

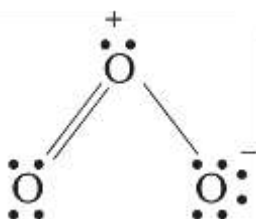
- The formal charge on end O atom number 2:

$$= 6 - 4 - \frac{1}{2}(4) = 0$$

- The formal charge on end O atom number 3:

$$= 6 - 6 - \frac{1}{2}(2) = -1$$

The formal charge on O_3 molecule is as follows:



- The formal charge is based on a pure covalent view of bonding in which electron pairs are shared equally by neighboring atoms.

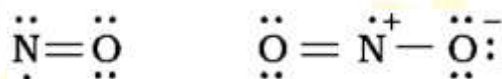
Limitations of octet rule

- There are some exceptions to the octet rule
- The incomplete octet of the central atom** – The number of electrons surrounding central atom is less than 8. In case of elements having four or less valence electrons. Example: LiCl, BeH₂, BCl₃.

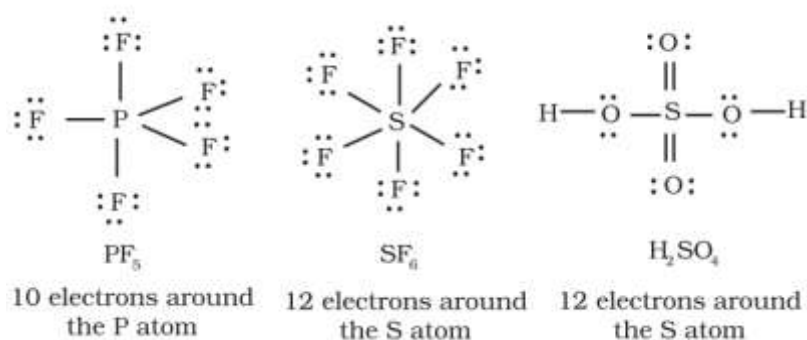


Here Li has 1, Be has 2 and B has 3 valence electrons.

- Odd-electron molecules** – Some molecules with an odd number of electrons. For example: nitric oxide, nitrogen oxide, the octet rule is not satisfied for all such atoms.



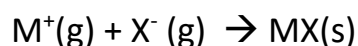
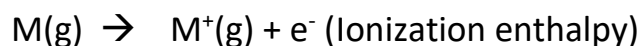
- The expanded octet** – Some elements have more than 8 valence e⁻ around the central atom, which is known as expanded octet. Examples: PF₅, H₂SO₄, SF₆.



- Octet rule is based on chemical inertness of noble gases while some noble gases like Xe, Kr combine with fluorine and oxygen to form a number of compounds like XeOF₂, XeF₂, KrF₂.
- Octet rule failed to describe the relative stability of the molecules.
- Octet rule cannot explain the shape of molecule.

Ionic or electrovalent bond

- The formation of ionic compounds depends upon the ease of formation of negative and positive ions from the representative neutral atoms; also, on the arrangement of negative and positive ions in the lattice of crystalline solid.



- The electron gain enthalpy ($\Delta_{eg}H$) is the enthalpy change when a gas phase atom in its ground state gains an electron. It can be exothermic or endothermic process. Ionization is an endothermic process.
- Ionic bonds form easily between elements with low ionization enthalpies and elements with high negative value of electron gain enthalpy.
- Ionic compounds are crystalline solids with 3-d arrangement of cations and anions.

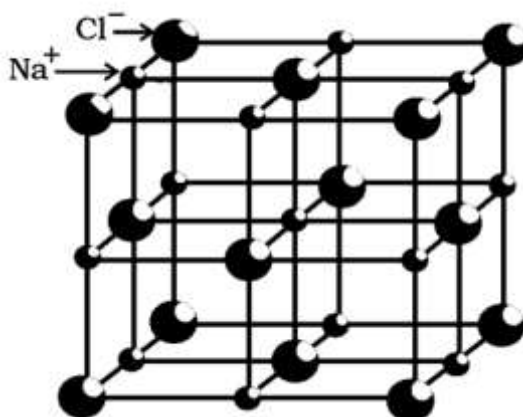


Figure: Rock salt structure

- The ionization enthalpy for Na⁺ from Na(g) = 495.8 KJ mol⁻¹
- The electron gain enthalpy for
 $Cl(g) + e^- \rightarrow Cl^-(g) \quad -348.7 \text{ KJ mol}^{-1}$

- $-348.7 + 495.8 = 147.1 \text{ KJ mol}^{-1}$

It is more than the enthalpy of lattice formation i.e., -788 KJ mol^{-1} . Thus, energy will be released.

Lattice energy

- The amount of energy required to separate one mole of a solid ionic compound into gaseous constituent ions is called lattice energy.
- The lattice energy of NaCl is 788 KJ mol^{-1} .

Bond Parameters

1. Bond length

- The equilibrium distance between the nuclei of two bonded atoms in a molecule is called bond length.
- The radius of an atom which is in contact with the core of an adjacent atom in a bonded atom is known as covalent radius.

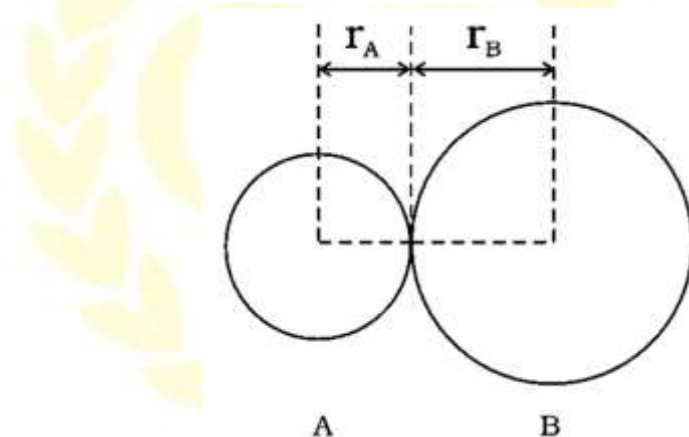


Figure: The bond length in a covalent molecule AB

- The van der Waals radius represents overall size of the atom which includes valence shell in a non-bonded situation.

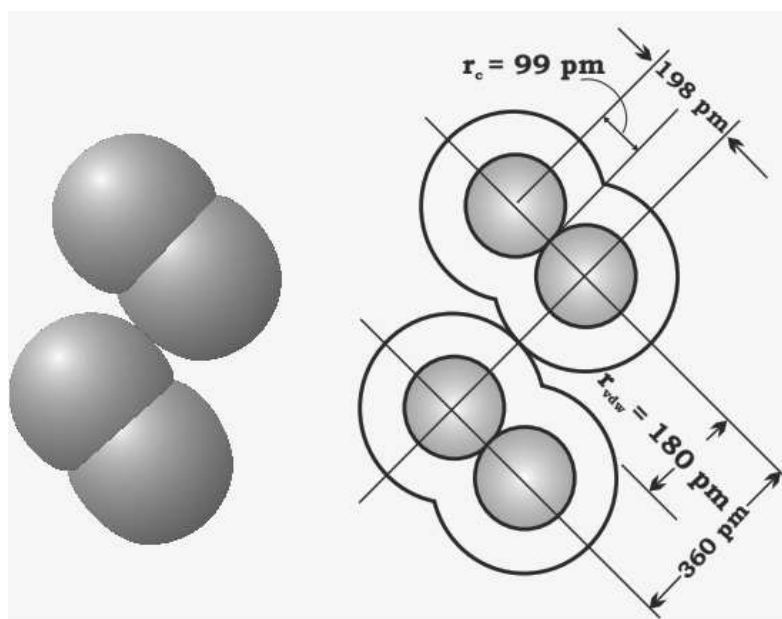
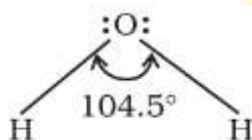


Figure: Covalent and van der Waals radius in chlorine molecule

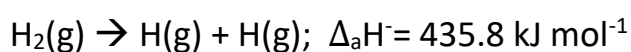
2. Bond Angle –

- The angle between the orbitals containing bonding electron pairs around the central atom in molecule is known as bond angle.
- It is expressed in degree.
- Example: Bond angle in water (H_2O)

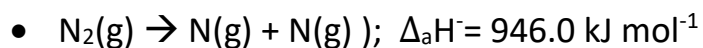


3. Bond Enthalpy –

- The amount of energy required to break 1 mole bonds between two atoms in gaseous state is known as bond enthalpy.
- The unit of bond enthalpy is kJ mol^{-1} .
- The bond enthalpy for H-H bond is 435 kJ mol^{-1} .

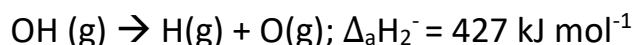
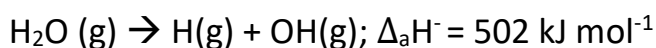


- $\text{O}_2(\text{g}) \rightarrow \text{O}(\text{g}) + \text{O}(\text{g}); \Delta_a H^\circ = 498 \text{ kJ mol}^{-1}$



Thus, we can say the stronger the bond, larger the bond dissociation enthalpy of a molecule.

- Heteronuclear diatomic molecule like hydrochloric acid (HCl) –
 $\text{HCl}(\text{g}) \rightarrow \text{H}(\text{g}) + \text{Cl}(\text{g})$; $\Delta_{\text{a}}H^\ominus = 431.0 \text{ kJ mol}^{-1}$
- Bond strength is complicated in case of polyatomic molecules. Like in water molecule, two O-H bond enthalpies are not similar.



The different $\Delta_{\text{a}}H^\ominus$ value shows that there is some different chemical environment around second O-H bond.

For O-H bond mean or average bond enthalpy =

$$= \frac{502 + 427}{2} = 464.5 \text{ kJ mol}^{-1}$$

Table: Average bond length for some bonds

Bond Type	Covalent Bond Length (pm)
O-H	96
C-H	107
N-O	136
C-O	143
C-N	143
C-C	154
C=C	121
N=O	122
C=C	133
C=N	138
C≡N	116
C≡C	120

Table: Bond lengths in some molecules

Molecules	Bond Length (pm)
H ₂ (H-H)	74
F ₂ (F-F)	144
Cl ₂ (Cl-Cl)	199
Br ₂ (Br-Br)	228
I ₂ (I-I)	267
N ₂ (N≡N)	109
O ₂ (O=O)	121
HF (H-F)	92
HCl (H-Cl)	127
HBr (H-Br)	141
HI (H-I)	160

4. Bond Order

- The number of bonds between two atoms is known as bond order. Examples: In H₂, O₂ and N₂ the bond order is 1, 2, and 3 respectively.
- Isoelectronic molecules and ions have identical bond orders. Examples: F₂ and O₂²⁻ have 1 bond order. CO, N₂ and NO₊ have bond order 3.

$$\diamond \text{ Bond order} \propto \text{Bond energy} \propto 1/\text{Bond length}$$

Resonance structure

- Sometimes Lewis structure is not sufficient for the representation of a molecule. For example, ozone molecule can be represented by these structures as shown in figure below.
- Here structure I and II are canonical forms and structure III is resonance hybrid.

- In O_3 molecule O-O single bond's bond length is 148 pm and O=O bond length is 121 pm. But experimentally O-O bond length in O_3 molecule is 128 pm. Thus, it is intermediate between single and double bond. It is not possible to represent it by Lewis's structure.

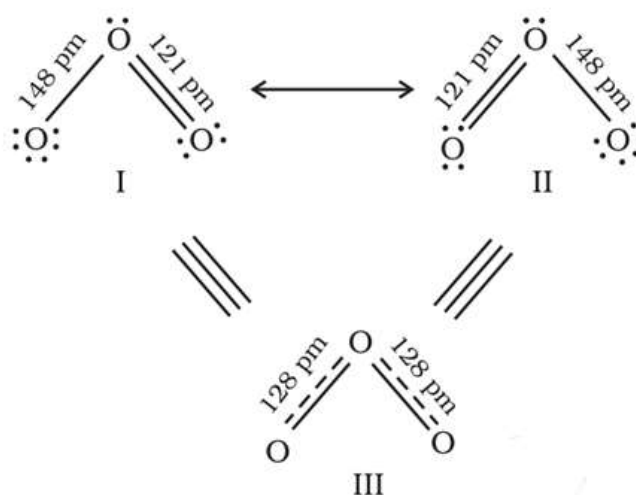


Figure: Resonance in O_3 molecule

- A single Lewis structure cannot describe well a molecule.
- A number of structures with similar position of nuclei; energy, non-bonding and bonding pairs of electrons are taken as the canonical structures of the resonance hybrid which describe well and accurately the molecule.
- Resonance is represented by double headed arrow.
- For example, in carbon di oxide (CO_2) molecule –

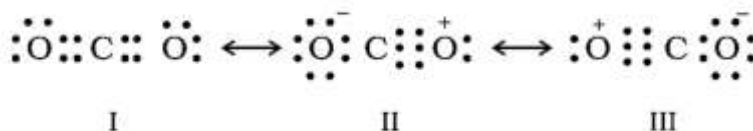


Figure: resonance in CO_2 molecule, I, II and III represent the three canonical structures.

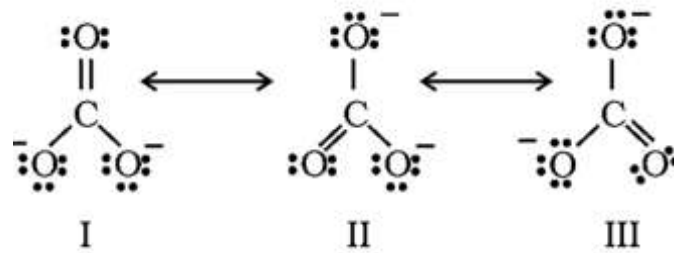


Figure: Resonance in CO_3^{2-} , I, II and III represent the three canonical forms.

- ❖ The energy of resonance hybrid is less than the energy of a single canonical structure thus resonance stabilizes the molecule.
- ❖ As a whole, the bond characteristics are made average by resonance.
- ❖ **Misconceptions**
 1. The canonical forms have no real existence.
 2. The molecule does not exist for a certain period of time in one canonical form.
 3. There is no equilibrium between the canonical forms as in tautomerism.

Polarity in bonds

- There is no bond or compound is completely ionic or covalent.
- When the shared pair of electrons is equally attracted by two atoms, the formation of covalent bond take place. And it is known as non-polar covalent bond. For example, in H_2 , Cl_2 , O_2 and F_2 .
Thus, the electron pair is situated exactly between the identical nuclei. And it is known as non-polar covalent bond.
- In Heteronuclear molecule the shared pair of electrons is situated towards more electronegative atom. Like in HF towards fluorine. It is known as polar covalent bond.
- Difference in electronegativity causes the polarization. Due to this polarization, molecule possesses dipole moment.

- **Dipole moment-** The product of magnitude of the charge and distance between centers of negative and positive charge is known as dipole moment.
- Dipole moment is denoted by μ .

Dipole moment (μ) = charge (Q) x distance of separation(r)

$$\mu = Qr$$

- Unit of dipole moment is **Debye**.

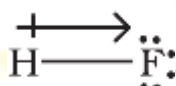
$$1D = 3.3356 \times 10^{-30} \text{ C m}$$

Here C is coulomb and m is meter.

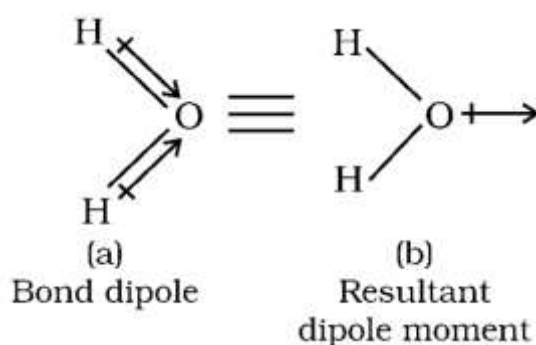
- It is a vector quantity depicted by



The tail lies on the electronegative center. For example

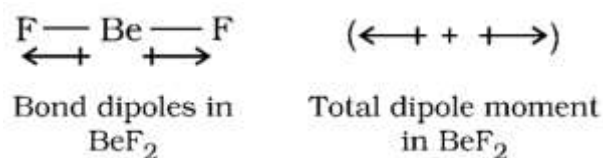


- The arrow shows the direction of the shift of electron density in the molecule.
- In polyatomic molecules dipole moment depends upon the individual dipole moments of bonds. For example, in water molecule –



H₂O has bent structure, and bond angle is 104.5°. Net dipole moment is $6.17 \times 10^{-30} \text{ C m}$.

- In case of BeF₂ net dipole moment is zero because two equal dipole moment lies in opposite directions. They cancel the dipole moment of each other.



- In tetra-atomic molecule like BF_3 the net dipole moment is zero. As the bond angle is 120° . The dipole moment of middle one and resultant dipole moment of other two sides, cancel each other.

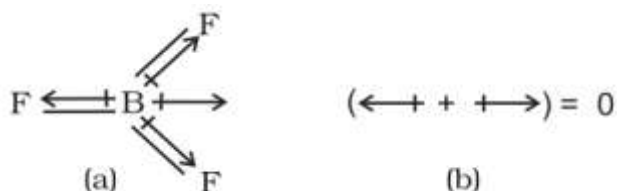
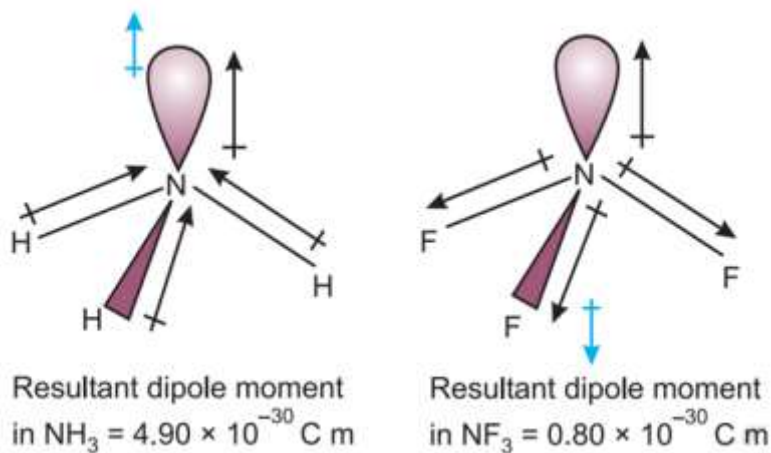


Figure: (a) Bond dipoles (b) Total dipole moment

- In presence of lone pair, the calculation of dipole moment is more interesting. For example, in NH_3 and NF_3 .
- In NH_3 the orbital dipole due to lone pair is in the same direction as the resultant dipole moment of N-H bonds.
- In NF_3 the orbital dipole is in the opposite direction to the resultant dipole moment. Thus, NF_3 has low dipole moment as compare to NH_3 .



(Here blue colored arrow show resultant dipole moment)

Fajans Rule – The partial covalent character in ionic bond was discussed by Fajans rule. According to this rule –

1. $\frac{\text{Size of anion}}{\text{Size of cation}} \propto \text{Covalent character of an ionic bond}$

2. **Charge on cation** \propto **Covalent character of an ionic bond**

3. In case of cations with similar size and charge, the one with $(n-1)d^nns^0$ (transition metals) is more polarizing than the one with noble gas configuration i.e. ns^2np^6 .

The cation polarizes the anion by pulling the electronic charge towards itself. Eventually the electronic charge increases between the two.

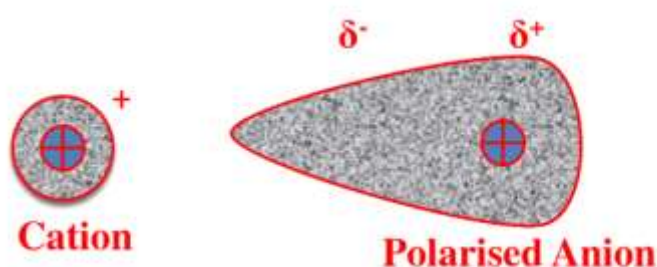


Figure: Polarization of anion by cation

Examples: Sodium chloride (NaCl) (with a low positive charge (+1), a fairly large cation ($\sim 1 \text{ \AA}$) and relatively small anion (0.2 \AA) is ionic; but Aluminum iodide (AlI_3) (Al with a high positive charge (+3) and a large anion I^-) is covalent.

The valence shell electron pair repulsion theory (VSEPR) –

- Sidgwick and Powell in 1940 formulated this theory which is based on repulsive interactions of the electron pairs in the valence shell of the atoms.
- It was further improvised by Nyholm and Gillespie in 1957.

The main postulates of VSEPR theory:

- The shape of a molecule completely depends upon the number of valence shell electron pairs (bonded or non-bonded) present around the central atom.
- Pairs of electrons in the valence shell repel one another since their electron clouds are negatively charged.

- These pairs of electrons tend to occupy such positions in space that minimize repulsion and maximize the distance between them.
- The valence shell is taken as a sphere with the electron pairs situated on the spherical surface at maximum distance from one another.
- A multiple bond is treated as if it is a single electron pair and two or three electron pairs of a multiple bond are treated as a single super pair.
- Where two or more resonance structures can represent a molecule, the VSEPR model is applicable to any such structure.

❖ The repulsive interaction of electron pairs decreases in the order:

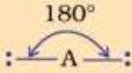
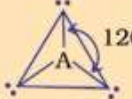
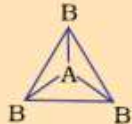
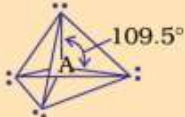
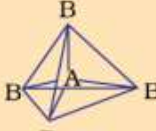
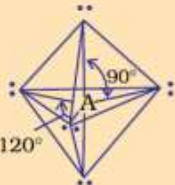
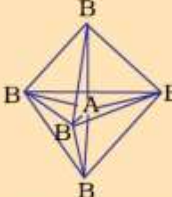
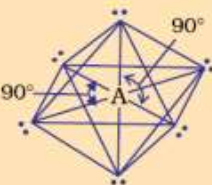
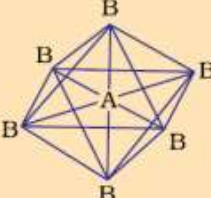


Here lp = lone pair

bp = bond pair

- Nyholm and Gillespie improvised the VSEPR model by explaining the important difference between the lp and bp of electrons.
- The lone pairs are localized on the central atom. The bond pair is shared between two atoms. Thus, the lone pair of electrons in a molecule occupy more space as compared to the bonding pairs of electrons. This results in repulsion between lone pairs of electrons as compared to lp - bp and bp - bp repulsions. These repulsive effects result in deviations from ideal shapes and changes in bond angles in molecules.
- The VSEPR theory divides molecules into two categories:
 1. Molecules in which the central atom has no lone pair
 2. Molecules in which the central atom has one or more lone pairs.

Table: Geometry of Molecules in which the Central Atom has No Lone Pair of Electrons

Number of electron pairs	Arrangement of electron pairs	Molecular geometry	Examples
2	 <p>180° Linear</p>	<p>B—A—B Linear</p>	BeCl ₂ , HgCl ₂
3	 <p>120° Trigonal planar</p>	 <p>Trigonal planar</p>	BF ₃
4	 <p>109.5° Tetrahedral</p>	 <p>Tetrahedral</p>	CH ₄ , NH ₄ ⁺
5	 <p>90° 120° Trigonal bipyramidal</p>	 <p>Trigonal bipyramidal</p>	PCl ₅
6	 <p>90° 90° Octahedral</p>	 <p>Octahedral</p>	SF ₆

- The compounds of AB₂, AB₃, AB₄, AB₅ and AB₆, the arrangement of electron pairs and the B atoms around the central atom A are : linear, trigonal planar, tetrahedral, trigonalbipyramidal and octahedral, respectively.
- Such arrangements can be seen in the molecules like BF₃(AB₃), CH₄ (AB₄) and PCl₅ (AB₅) as shown below by their ball and stick models-

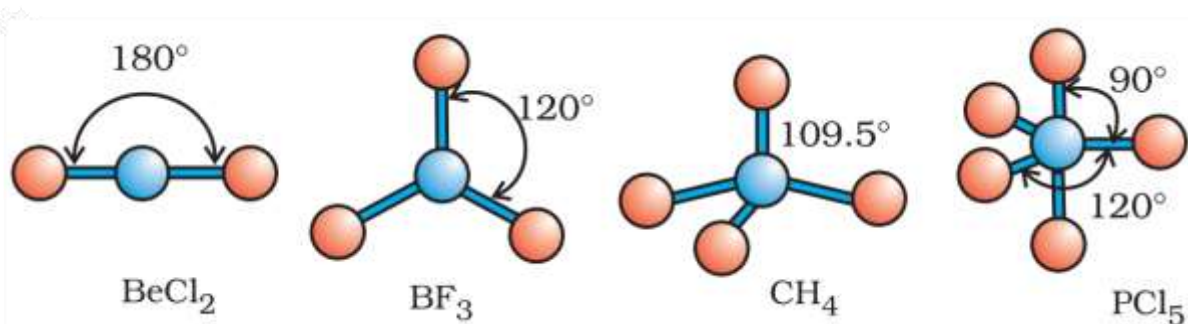


Figure: the shape of molecules in which central atom has no lone pair

- The VSEPR Theory is able to predict geometry of a large number of molecules, especially the compounds of p-block elements accurately.
- It is also quite successful in determining the geometry very accurately even when the energy difference between possible structures is very small.



Table: Geometry of Molecules in which the Central Atom has No Lone Pair of Electrons

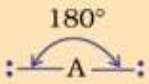
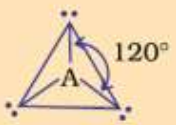
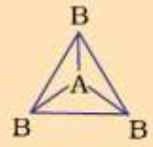
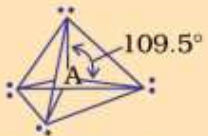
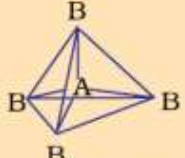
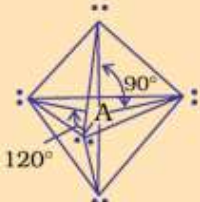
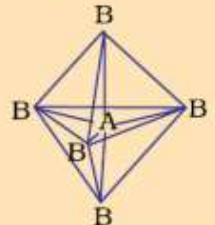
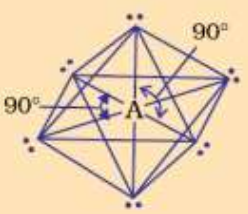
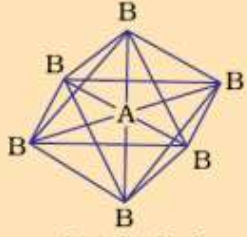
Number of electron pairs	Arrangement of electron pairs	Molecular geometry	Examples
2	 <p>180° :—A—: Linear</p>	B—A—B Linear	BeCl ₂ , HgCl ₂
3	 <p>120° Trigonal planar</p>	 <p>Trigonal planar</p>	BF ₃
4	 <p>109.5° Tetrahedral</p>	 <p>Tetrahedral</p>	CH ₄ , NH ₄ ⁺
5	 <p>90° 120° Trigonal bipyramidal</p>	 <p>Trigonal bipyramidal</p>	PCl ₅
6	 <p>90° 90° Octahedral</p>	 <p>Octahedral</p>	SF ₆

Table: Shape (geometry) of some simple molecules/ions with central ions having one or more lone pairs of electrons (E).

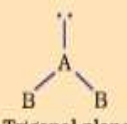
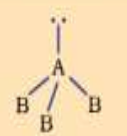
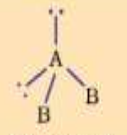
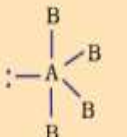


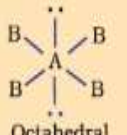
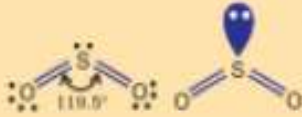
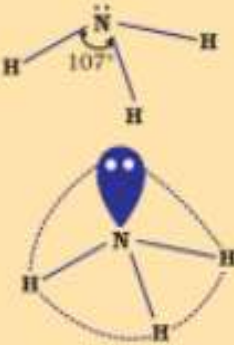
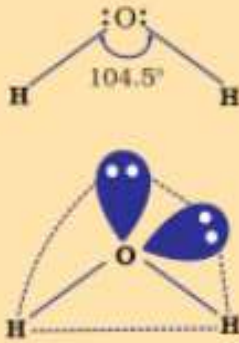
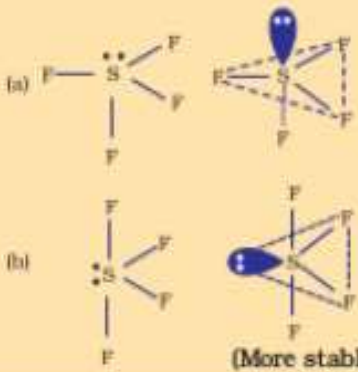
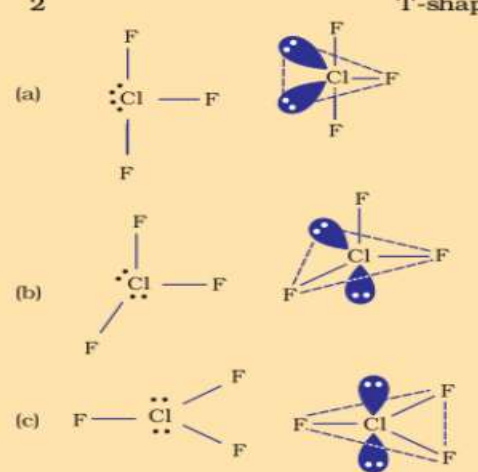
Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electron pairs	Shape	Examples
AB_2E	2	1	 <p>Trigonal planar</p>	Bent	SO_2, O_3
AB_3E	3	1	 <p>Tetrahedral</p>	Trigonal pyramidal	NH_3
AB_2E_2	2	2	 <p>Tetrahedral</p>	Bent	H_2O
AB_4E	4	1	 <p>Trigonal bi-pyramidal</p>	See saw	SF_4
AB_3E_2	3	2	 <p>Trigonal bi-pyramidal</p>	T-shape	ClF_3
AB_5E	5	1	 <p>Octahedral</p>	Square pyramid	BrF_5
AB_4E_2	4	2	 <p>Octahedral</p>	Square planar	XeF_4

Table: Shapes of molecules containing bond pair and lone pair

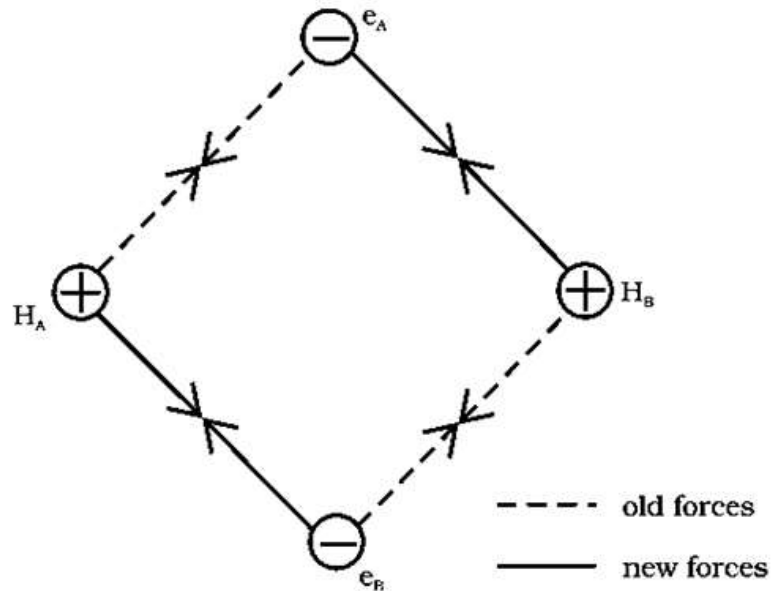
Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electrons	Shape	Reason for the shape acquired
AB_3E	4	1		Bent	Theoretically the shape should have been triangular planar but actually it is found to be bent or v-shaped. The reason being the lone pair-bond pair repulsion is much more as compared to the bond pair-bond pair repulsion. So the angle is reduced to 119.5° from 120° .
AB_3E	3	1		Trigonal pyramidal	Had there been a bp in place of lp the shape would have been tetrahedral but one lone pair is present and due to the repulsion between lp-bp (which is more than bp-bp repulsion) the angle between bond pairs is reduced to 107° from 109.5° .
AB_2E_2	2	2		Bent	The shape should have been tetrahedral if there were all bp but two lp are present so the shape is distorted tetrahedral or angular. The reason is lp-lp repulsion is more than lp-bp repulsion which is more than bp-bp repulsion. Thus, the angle is reduced to 104.5° from 109.5° .
AB_4E	4	1		See-saw	In (a) the lp is present at axial position so there are three lp-bp repulsions at 90° . In (b) the lp is in an equatorial position, and there are two lp-bp repulsions. Hence, arrangement (b) is more stable. The shape shown in (b) is described as a distorted tetrahedron, a folded square or a see-saw.

Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electrons	Shape	Reason for the shape acquired
AB_3E_2	3	2		T-shape	In (a) the lp are at equatorial position so there are less lp-bp repulsions as compared to others in which the lp are at axial positions. So structure (a) is most stable. (T-shaped).

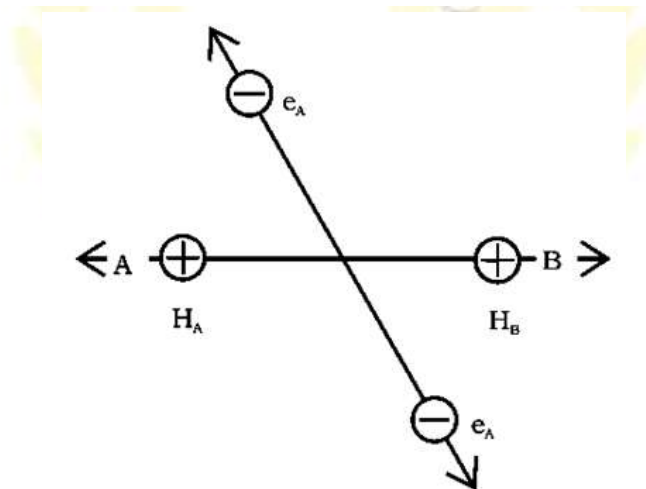
Valence bond theory –

- Valence bond theory was propounded by Heitler and London in 1927.
- It is based on atomic orbitals, electronic configurations of elements, overlapping of atomic orbitals, hybridization of atomic orbitals and principles of superposition and variation.
- Two hydrogen atoms A and B approaching each other having nuclei N_A and N_B and electrons present in them are represented by e_A and e_B .
- When the two atoms are at large distance from each other, there is no interaction between them. As these two atoms approach each other, new attractive and repulsive forces begin to operate.
- Attractive forces arise between them:
 1. Nucleus of one atom and its own electron i.e. $N_A - e_A$ and $N_B - e_B$.
 2. Nucleus of one atom and electron of other atom i.e. $N_A - e_B$, $N_B - e_A$.
- Repulsive forces arise between them:

1. Electrons of two atoms like $e_A - e_B$,
2. Nuclei of two atoms $N_A - N_B$.



Attractive Forces

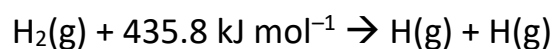


Repulsive Forces

Figure: Forces of attraction and repulsion during the formation of H₂ molecule

- Attractive forces bring the two atoms closer to each other while repulsive forces push them apart.
- The net force of attraction balances the force of repulsion and system acquires minimum energy. Thus, two hydrogen atoms bonded together. They make a stable molecule with bond length 74 pm.

- The energy released during bond formation is known as bond enthalpy. 435.8 kJ of energy is required to dissociate 1 mole of H₂ molecule.

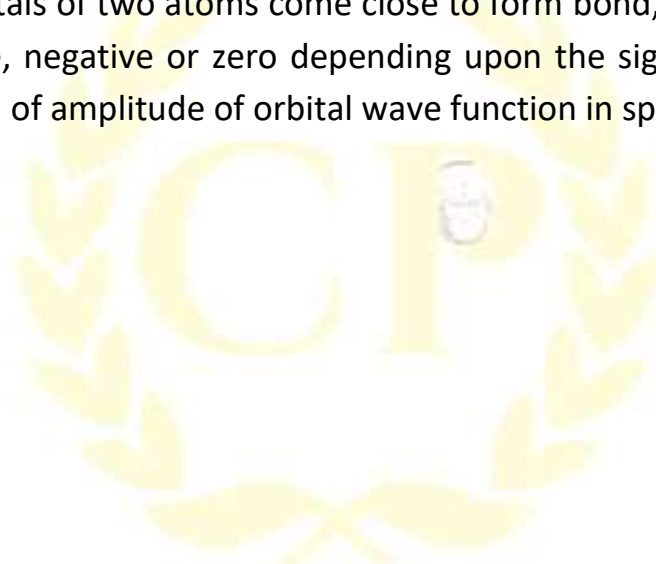


Orbital overlap concept –

- The partial merging of atomic orbitals is known as overlapping of atomic orbitals; which results in pairing of electrons.
- The strength of a covalent bond is decided by the extent of overlap.

Overlapping of atomic orbitals

- When orbitals of two atoms come close to form bond, their overlap may be positive, negative or zero depending upon the sign and direction of orientation of amplitude of orbital wave function in space.



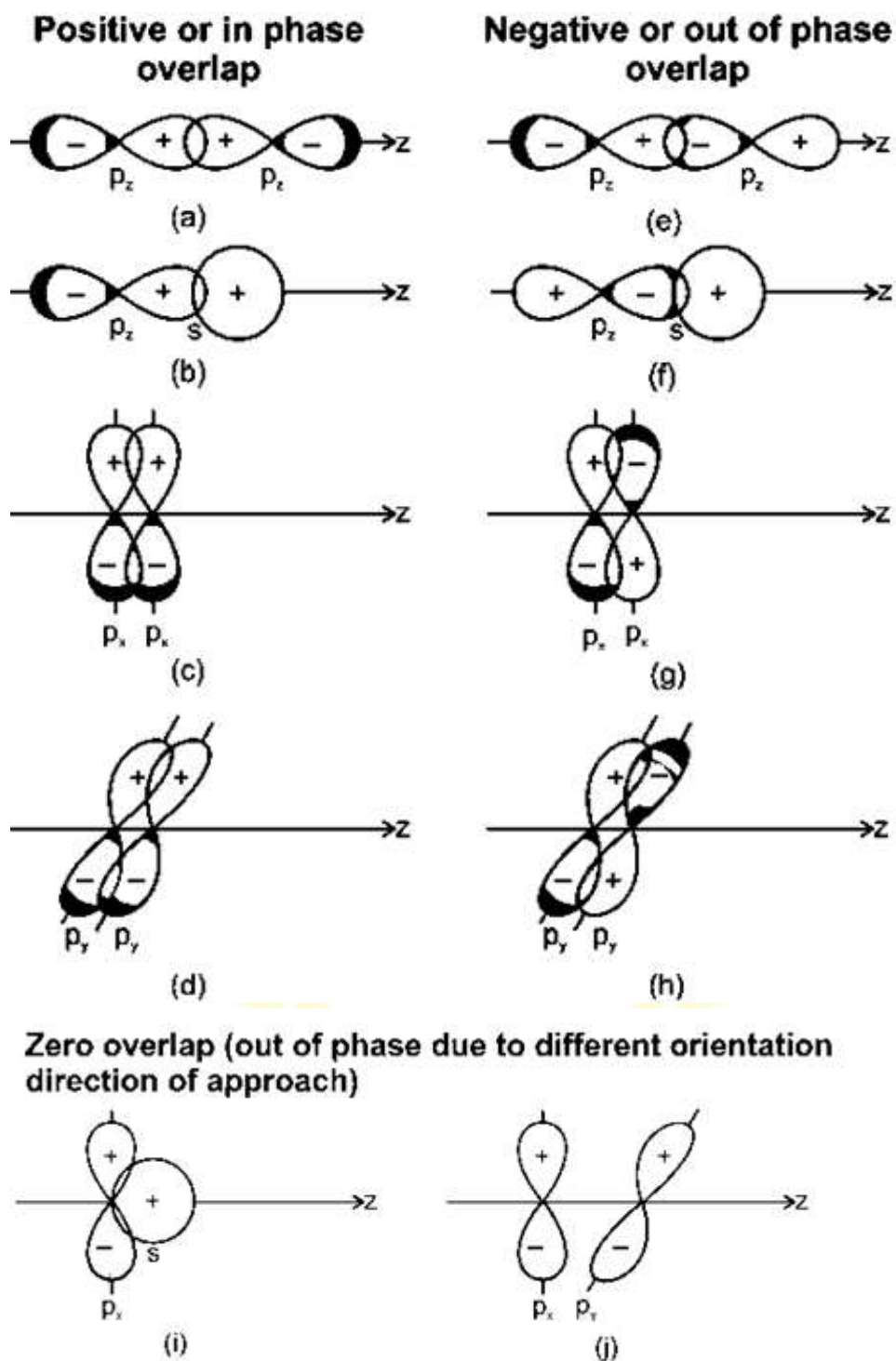


Figure: positive, negative and zero overlap of s and p atomic orbitals

- Orbitals forming bond should have same sign/phase and orientation in space. This is called positive overlap.
- The shapes of CH_4 , NH_3 , and H_2O molecules are tetrahedral, pyramidal and bent respectively. Valence bond theory explains the geometrical shapes in terms of the orbital overlaps.

- For example, in methane (CH_4) –
Electronic configuration of Carbon - $[\text{He}]2s^22p^2$
Electronic configuration of excited state - $[\text{He}] 2s^1 2px^1 2py^1 2pz^1$.
- Here the energy required for excitation is compensated by the release of energy due to overlap between the orbitals of carbon and hydrogen.
- The 4 atomic orbitals of carbon, each with an unpaired electron can overlap with the 1s orbitals of the four H atoms which are also singly occupied. This will result in the formation of four C-H bonds.
- The three p orbitals of carbon are at 90° to one another, the HCH angle for these will also be 90° . Three C-H bonds will be oriented at 90° to one another. The 2s orbital of carbon and the 1s orbital of H are spherically symmetrical and they can overlap in any direction.
- Simple atomic orbital overlap does not account for the directional characteristics of bonds in CH_4 . The tetrahedral HCH angles of 109.5°
- In case of NH_3 and H_2O molecules, the HNH and HOH angles should be 90° . But the actual bond angles are 107° and 104.5° in the NH_3 and H_2O molecules respectively.

Types of overlapping and nature of covalent bond

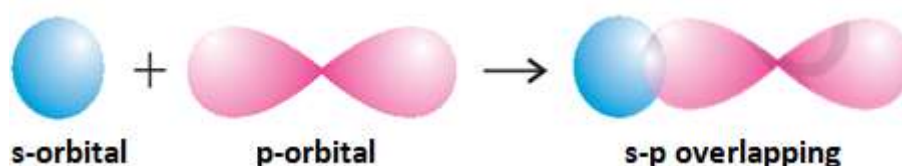
- The covalent bond is classified into two types depending upon the types of overlapping: **Sigma (σ) and pi (π)**

1. Sigma (σ) bond:

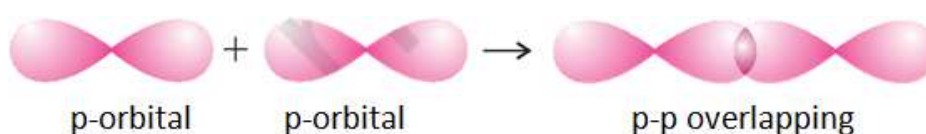
- Sigma bond is formed by the end-to-end overlap of bonding orbitals along the internuclear axis.
- This is called as head on overlap or axial overlap. This can be formed by any one of the following types of combinations of atomic orbitals:
 - A) s-s overlapping: In this overlapping, overlap of two half-filled s – orbitals along the internuclear axis take place.



B) **s-p** overlapping: This type of overlapping takes place between half-filled s- orbital and p-orbital.

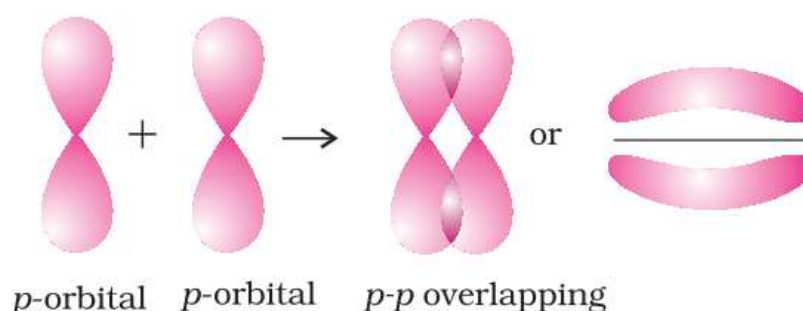


C) **p-p** overlapping: This type of overlap takes place between half-filled p-orbitals of the two approaching atoms.



2. Pi(π) bond:

- In the formation of π bond the atomic orbitals overlap in such a way that their axes remain parallel (\parallel) to each other and perpendicular (\perp) to the internuclear axis.
- The orbitals formed due to sidewise overlapping consists of two saucer type charged clouds above and below the plane of the participating atom.



Strength of Sigma and pi Bonds –

- The strength of a bond depends upon the extent of overlapping.
- The overlapping of orbitals takes place to a larger extent in sigma bond formation so it is stronger as compared to the pi bond where the extent of overlapping occurs to a smaller extent.

Order of strength: σ bond > π bond

- The formation of multiple bonds between two atoms of a molecule, pi bond(s) is formed in addition to a sigma bond.

Hybridization –

- Pauling propounded the concept of hybridization.
- The atomic orbitals combine to form new set of equivalent orbitals called hybrid orbitals.
- Hybridization is the process of intermixing of the orbitals of different energies and formation of new set of orbitals of same energies and shape.

Salient features of hybridization

1. The number of hybrid orbitals is equal to the number of the atomic orbitals that get hybridized.
2. The hybridized orbitals are always same in energy and shape.
3. The hybrid orbitals are more effective in forming stable bonds than the pure atomic orbitals.
4. These hybrid orbitals are directed in space in some preferred direction to have minimum repulsion between electron pairs and thus a stable arrangement. Hybridisation indicates the geometry of the molecules.

Important conditions for hybridization

- a. The orbitals present in the valence shell of the atom are hybridized.
- b. The orbitals undergoing hybridization should have almost equal energy.
- c. Excitation of electron is not essential condition prior to hybridization.
- d. It is not necessary that only half-filled orbitals participate in hybridization. Sometimes filled orbitals of valence shell take part in hybridization.

Types of hybridization –

1. sp-hybridisation -

- This type of hybridization involves the mixing of one s and one p orbital resulting in the formation of two equivalent sp-hybrid orbitals.
- The suitable orbitals for sp-hybridization are s and p_z , if the hybrid orbitals are to lie along the z-axis.
- Each sp-hybrid orbital has 50% s-character and 50% p-character. Such a molecule in which the central atom is sp-hybridized and connected to other two central atoms has linear geometry.
- This type of hybridization is also known as diagonal hybridization.
- Example: **BeCl₂**

Electronic configuration of Be – $1s^2 2s^2$

Excited electronic configuration - $1s^2 2s^1 2p^1$

One 2s and one 2p orbital get hybridized and two sp-hybridized orbitals form. The angle is 180° .

The sp-hybridized orbital overlaps with the 2p-orbital of chlorine axially and forms two Be-Cl sigma bonds.

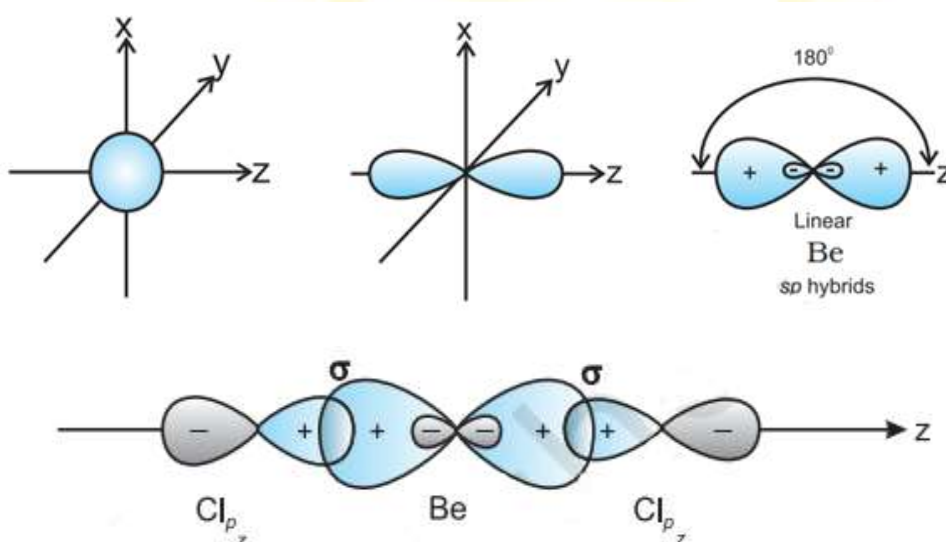


Figure: Formation of sp hybrids from s and p orbitals and formation of the linear BeCl₂ molecule

2. sp²-hybridization-

- In this hybridization there is involvement of one s and two p-orbitals in order to form three equivalent sp² hybridized orbitals.

- Example: BCl_3 molecule
 The ground state electronic configuration of central boron atom-
 $1s^2 2s^2 2p^1$
 The excited state electronic configuration of Boron atom-
 $1s^2 2s^2 2p_y^1 2p_z^1$
- In the excited state, one of the 2s electrons is promoted to vacant 2p orbital as a result boron has three unpaired electrons. These three orbitals (one 2s and two 2p) hybridize to form three sp^2 hybrid orbitals.

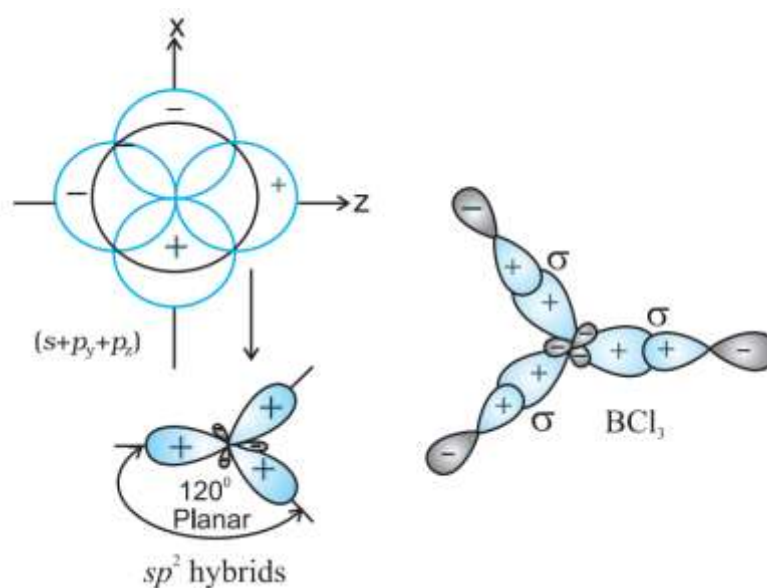


Figure: Formation of sp^2 hybrid and BCl_3 molecule

- The hybrid orbitals have a trigonal planar arrangement. The geometry is trigonal planar with Cl-B-Cl bond angle of 120° .

3. sp^3 - hybridization –

- This type of hybridization involves the mixing of one s-orbital and three p-orbitals of the valence shell to form four sp^3 -hybrid orbital of equivalent energies and shape.
- There is 25% s-character and 75% p-character in each sp^3 -hybrid orbital. The four sp^3 -hybrid orbitals so formed are directed towards the four corners of the tetrahedron.
- Example: CH_4 molecule

The ground state electronic configuration of central carbon atom-
 $1s^2 2s^2 2p^2$

- The excited state electronic configuration of carbon atom-
 $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$
- The angle between sp^3 -hybrid orbitals is 109.5° .

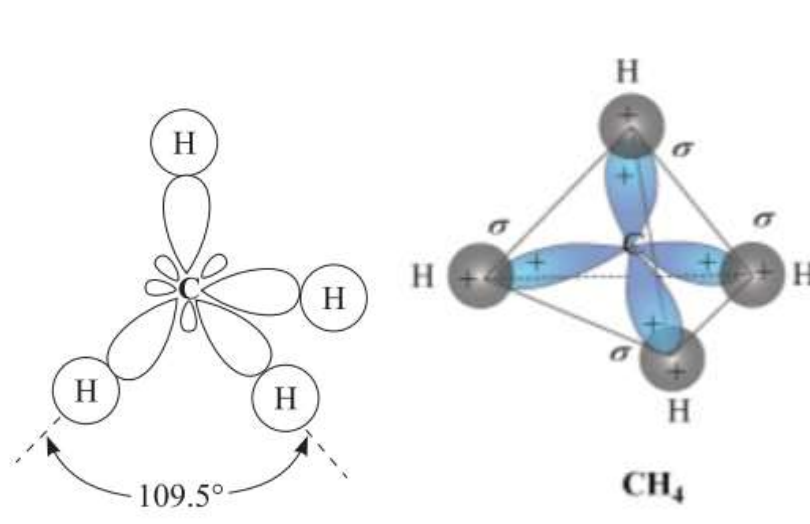


Figure: Formation of sp^3 -hybrid orbitals, formation of CH_4 molecule

- The structure of NH_3 and H_2O molecules can also be explained with the help of sp^3 -hybridization.
- **NH_3** – The valence shell (outer) electronic configuration of nitrogen atom in ground state- $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$
- There are three unpaired electrons in the sp^3 hybrid orbitals and a lone pair of electrons is present in the fourth one. These three hybrid orbitals overlap with $1s$ -orbitals of hydrogen atoms to form three N–H sigma (σ) bonds.
- There is a force of repulsion between a lone pair and a bond pair which is more than the force of repulsion between two bond pairs of electrons. The NH_3 molecule thus gets distorted and the bond angle is reduced to 107° from 109.5° . The geometry NH_3 molecule is pyramidal.

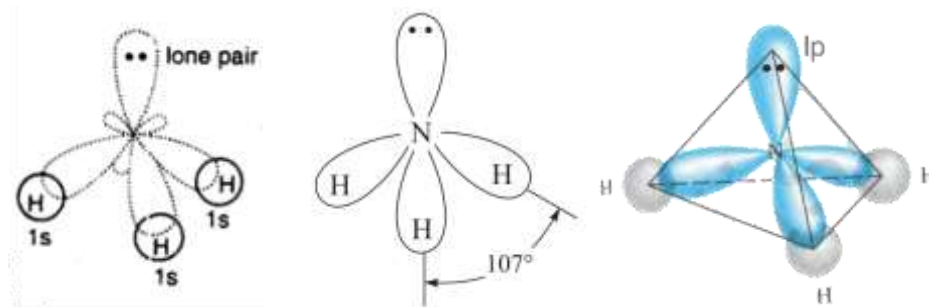


Figure: Formation of sp^3 -hybrid orbitals and formation of NH_3 molecule

- **H_2O** – The ground state electronic configuration of central oxygen atom- $1s^2 2s^2 2p^4$
- Four oxygen orbitals (one 2s and three 2p orbital) undergo sp^3 - hybridization forming four sp^3 -hybrid orbitals.
- Two of them contain one electron each and the other two contain a pair of electrons.
- These four sp^3 -hybrid orbitals acquire a tetrahedral geometry, with two corners occupied by H-atoms while the other two by the lone pairs.
- The bond angle in this case is reduced to 104.5° from 109.5° due to the presence of lone pair.
- Water molecule has V-shape or angular geometry.

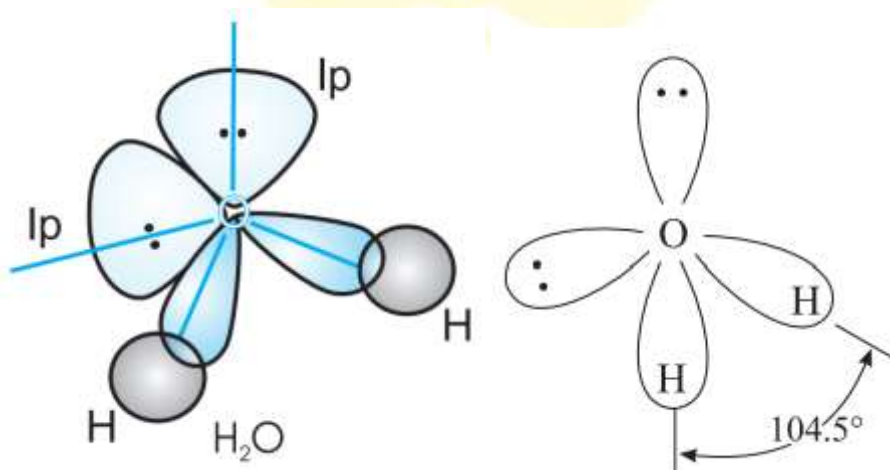


Figure: Orbital overlapping and formation of H_2O molecule

sp^3 -hybridization in C_2H_6 molecule:

- In ethane molecule both the carbon atoms assume sp^3 -hybrid state.
- One of the four sp^3 -hybrid orbitals of carbon atom overlaps axially with similar orbitals of other atom to form sp^3-sp^3 sigma (σ) bond while the other three hybrid orbitals of each carbon atom are used in forming sp^3-s sigma (σ) bonds with hydrogen atoms.
- C–C bond length is 154 pm and each C–H bond length is 110 pm.

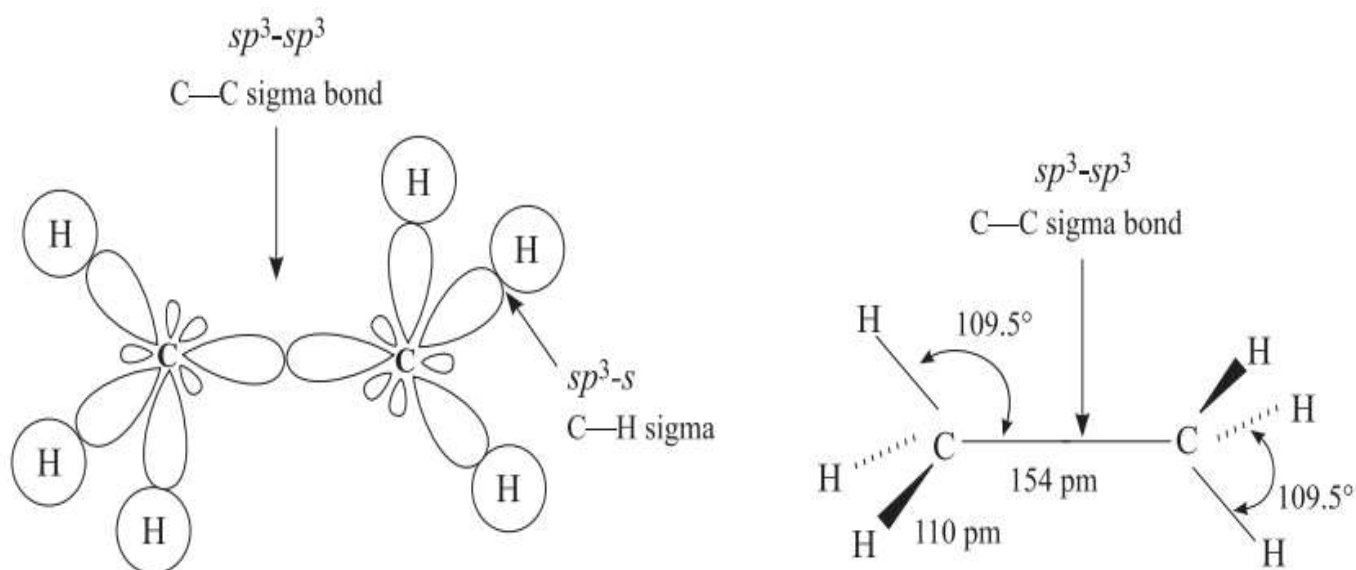


Figure: Orbital picture and structure of ethane

Sp^2 -hybridization in C_2H_4 molecule:

- In ethene molecule, one of the sp^2 -hybrid orbitals of carbon atom overlaps axially with sp^2 -hybridised orbital of another carbon atom to form C–C sigma bond.
- While the other two sp^2 -hybrid orbitals of each carbon atom are used for making sp^2-s sigma (σ) bond with two hydrogen atoms. The unhybridised orbital ($2p_x$ or $2p_y$) of one carbon atom overlaps sidewise with the similar orbital of the other carbon atom to form weak π bond; which consists of two equal electron clouds distributed above and below the plane of carbon and hydrogen atoms.

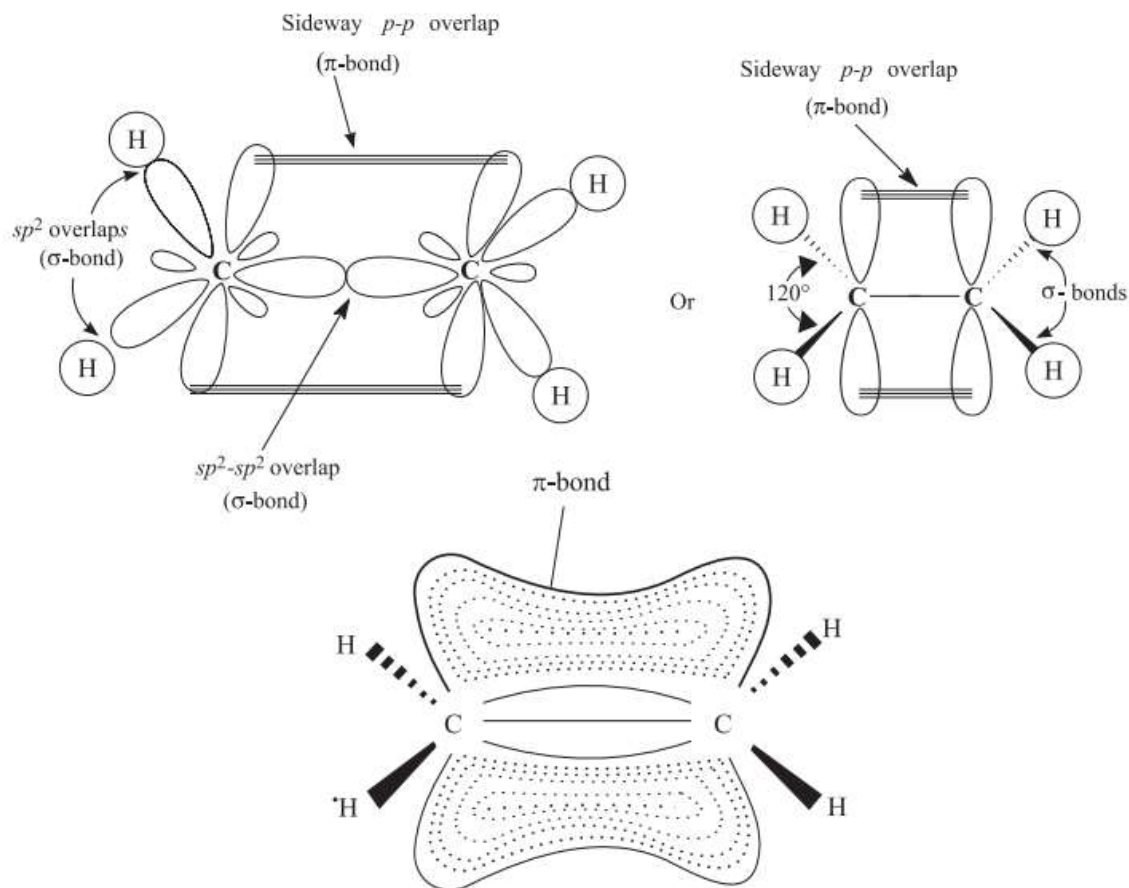


Figure: Orbital picture and structure of ethylene

sp-hybridization in C_2H_2 molecule:

- In ethyne molecule, both the carbon atoms undergo sp -hybridization having two unhybridized orbitals i.e., $2p_y$ and $2p_x$.
- One sp -hybrid orbital of one carbon atom overlaps axially with sp -hybrid orbital of the other carbon atom to form C–C sigma bond, while the other hybridized orbital of each carbon atom overlaps axially with the half-filled s -orbital of hydrogen atoms forming sigma bonds.
- Each of the two unhybridized p orbitals of both the carbon atoms overlaps sidewise to form two π bonds between the carbon atoms. So, the triple bond between the two carbon atoms is made up of one sigma and two pi bonds.

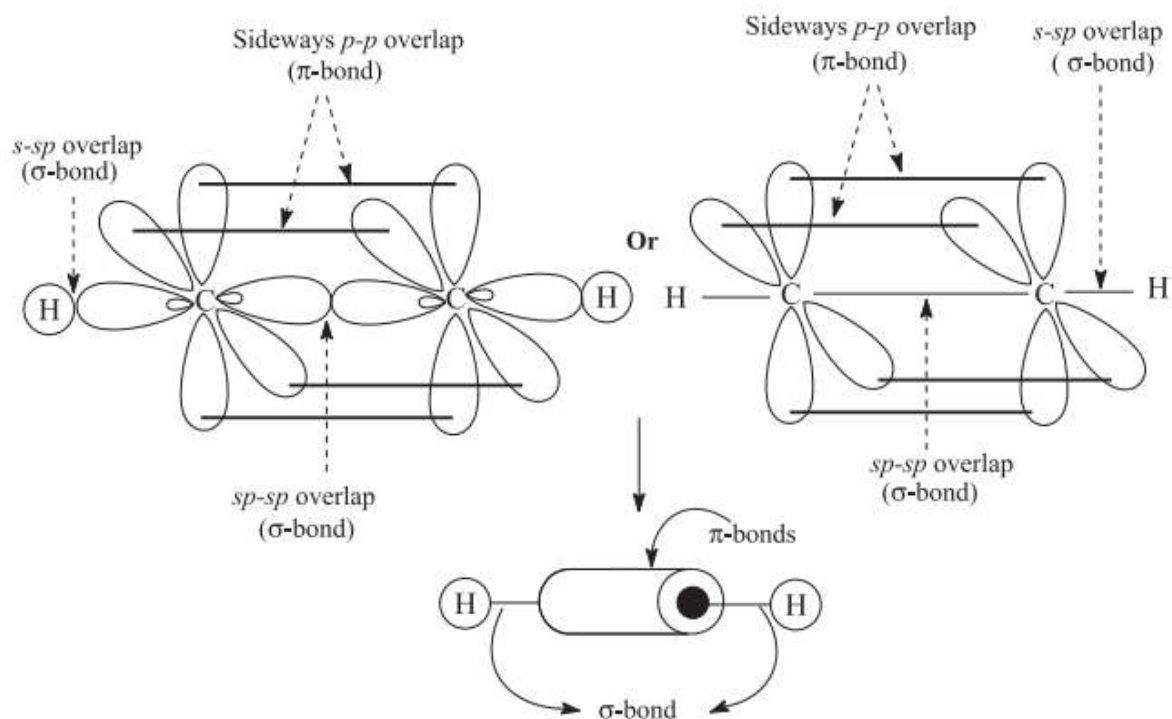


Figure: Formation of sigma and pi bond in ethyne

Hybridization of Elements involving d-Orbitals

- The elements present in the third period in periodic table contain d-orbitals in addition to s and p orbitals. The hybridization involving either 3s, 3p and 3d or 3d, 4s and 4p is possible. Hybridization involving 3p, 3d and 4s orbitals is not possible.

Table: Important hybridisation

Shape of molecules/ ions	Hybridisation type	Atomic orbitals	Example
Square planar	dsp^2	$d+s+p(2)$	$[Ni(CN)_4]^{2-}$ $[Pt(Cl)_4]^{2-}$
Trigonal bipyramidal	sp^3d	$s+p(3)+d$	PF_5, PCl_5
Square pyramidal	sp^3d^2	$s+p(3)+d(2)$	BrF_5
Octahedral	sp^3d^2 d^2sp^3	$s+p(3)+d(2)$ $d(2)+s+p(3)$	$SF_6, [CrF_6]^{3-}$ $[Co(NH_3)_6]^{3+}$

i) Formation of PCl_5 (sp^3d hybridization) –

The ground state and the excited state outer electronic configurations of phosphorus (Z=15) –

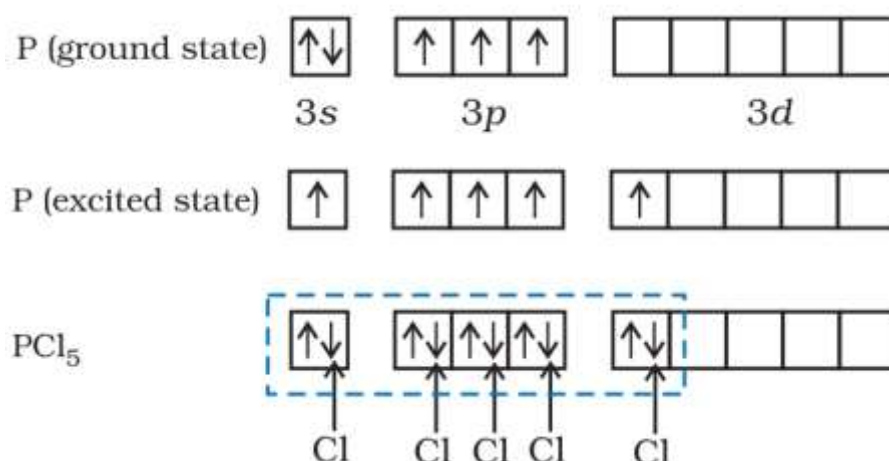


Figure: sp^3d hybrid orbitals filled by electron pairs donated by 5 Cl atoms

- The five orbitals (i.e., one s, three p and one d orbitals) are available for hybridization to yield a set of five sp^3d hybrid orbitals which are directed towards the five corners of a trigonal bipyramidal.

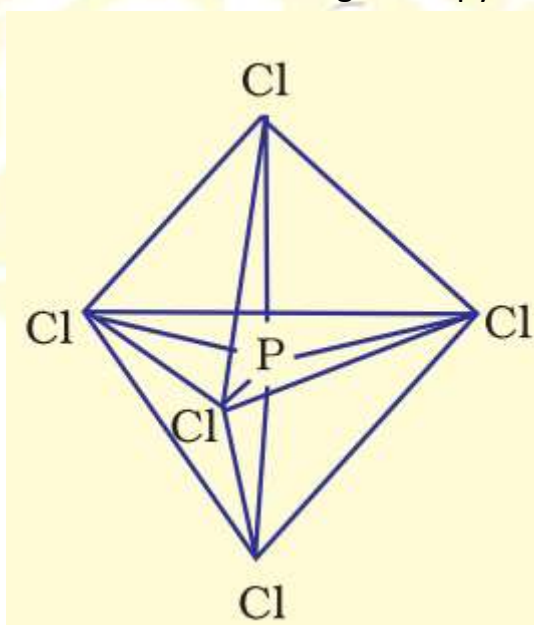


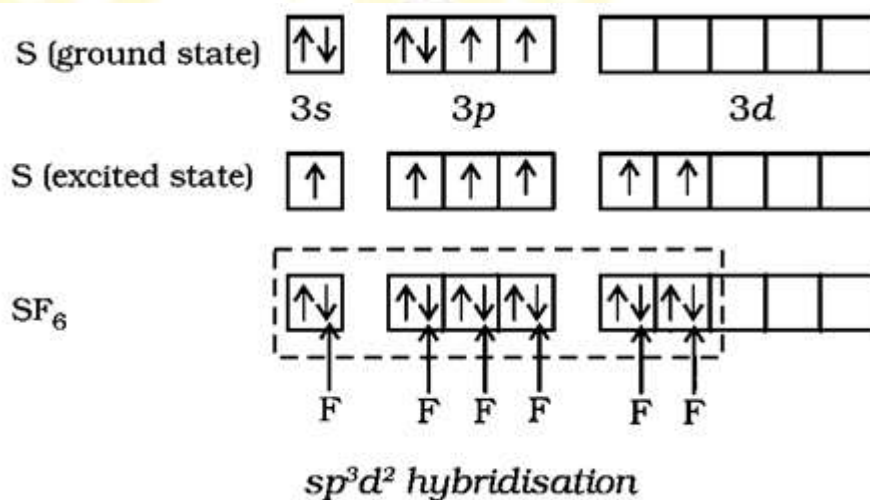
Figure: Trigonal bipyramidal geometry of PCl₅ molecule

- All the bond angles in trigonal bipyramidal geometry are not equivalent. In PCl₅ the five sp^3d orbitals of phosphorus overlap with the singly occupied p-orbitals of chlorine atoms to form five P–Cl sigma bonds.
- Three P–Cl bonds lie in one plane and make an angle of 120° with each other; these bonds are termed as equatorial bonds.

- The remaining two P–Cl bonds—one lying above and the other lying below the equatorial plane, make an angle of 90° with the plane.
- Axial bonds have been found to be slightly longer and hence slightly weaker than the equatorial bonds; which makes PCl_5 molecule more reactive.

ii) **Formation of SF_6 (sp^3d^2 hybridization)-**

- In SF_6 the central S-atom has the ground state outer electronic configuration - $3s^23p^4$
- In the excited state the available six orbitals i.e., one s, three p and two d are singly occupied by electrons. These orbitals hybridize to form six new sp^3d^2 -hybrid orbitals.
- These six sp^3d^2 hybrid orbitals overlap with singly occupied orbitals of fluorine atoms to form six S–F sigma bonds.
- SF_6 molecule has a regular octahedral geometry.



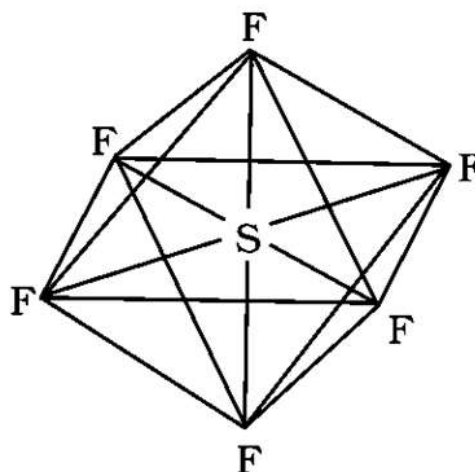


Figure: octahedral geometry of SF₆ molecule

MOLECULAR ORBITAL THEORY

- Molecular orbital theory was propounded by Hund and Mulliken in 1932.
- The salient features of this theory are:
 1. The electrons in a molecule are present in the various molecular orbitals as the electrons of atoms are present in the various atomic orbitals.
 2. The atomic orbitals of comparable energies and proper symmetry combine to form new molecular orbitals.
 3. An atomic orbital is monocentric while a molecular orbital is polycentric.
 4. The number of molecular orbitals formed is equal to the number of combining atomic orbitals. When two atomic orbitals combine, two molecular orbitals are formed. One is bonding molecular orbital while the other is called anti-bonding molecular orbital.
 5. The bonding molecular orbital has lower energy and greater stability than the corresponding anti-bonding molecular orbital.
 6. The electron probability distribution around a nucleus in an atom is given by an atomic orbital; the electron probability distribution around a group of nuclei in a molecule is given by a molecular orbital.
 7. The molecular orbitals are filled in accordance with the Aufbau principle obeying the Pauli's exclusion principle and the Hund's rule.

Formation of molecular orbitals: linear combination of atomic orbitals (LCAO)

- The atomic orbitals are expressed by wave functions (Ψ 's) which represent the amplitude of the electron waves. These are obtained from the solution of Schrodinger wave equation.
- In homo-nuclear diatomic H_2 molecule. Consider the H_2 molecule consisting of two atoms A and B. Each hydrogen atom in the ground state has one electron in 1s orbital.
- The atomic orbitals of these atoms may be represented by the wave functions Ψ_A and Ψ_B .
- The formation of molecular orbitals may be described by the linear combination of atomic orbitals as follows:

$$\Psi_{MO} = \Psi_A \pm \Psi_B$$

- The two molecular orbitals σ and σ^* are formed as follows:

$$\sigma = \Psi_A + \Psi_B$$

$$\sigma^* = \Psi_A - \Psi_B$$

- The molecular orbital σ formed by the addition of atomic orbitals is called the bonding molecular orbital and the molecular orbital σ^* formed by the subtraction of atomic orbital is called anti-bonding molecular orbital.

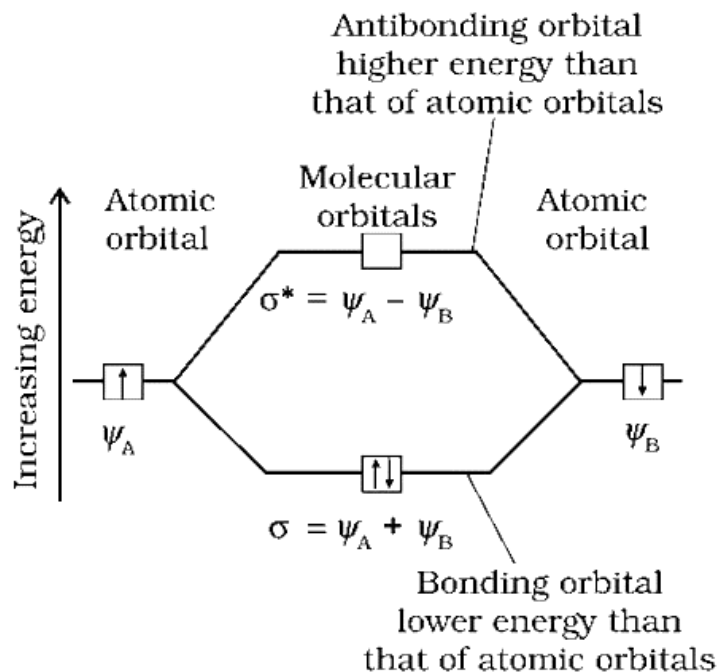


Figure: Formation of bonding (σ) and anti-bonding (σ^*) molecular orbitals by the linear combination of atomic orbitals ψ_A and ψ_B centered on two atoms A and B respectively.

- In the formation of bonding molecular orbital, the two electron waves of the bonding atoms reinforce each other due to **constructive interference**.
- In the formation of anti-bonding molecular orbital, the electron waves cancel each other due to **destructive interference**.
- The electron density in a bonding molecular orbital is located between the nuclei of the bonded atoms because of which the repulsion between the nuclei is very less while in case of an anti-bonding molecular orbital, most of the electron density is located away from the space between the nuclei.
- There is a nodal plane on which the electron density is zero. This nodal plane is situated between the nuclei and hence the repulsion between the nuclei is high.
- Electrons placed in a bonding molecular orbital tend to hold the nuclei together and stabilize a molecule. A bonding molecular orbital always possesses lower energy than either of the atomic orbitals that have combined to form it.

- The electrons placed in the anti-bonding molecular orbital destabilize the molecule. This is because the mutual repulsion of the electrons in this orbital is more than the attraction between the electrons and the nuclei, which causes a net increase in energy.
- The energy of anti-bonding orbital is elevated above the energy of the parent atomic orbitals that have combined and the energy of the bonding orbital has been lowered than the parent orbitals.

Conditions for the combination of atomic orbitals

1. The combining atomic orbitals must have nearly the same energy. This means that 1s orbital can combine with another 1s orbital but not with 2s orbital because the energy of 2s orbital is higher than that of 1s orbital. This is not true if the atoms are very different.
2. The combining atomic orbitals must have the same symmetry about the molecular axis. By convention z-axis is taken as the molecular axis. The atomic orbitals having same or nearly the same energy will not combine if they do not have the same symmetry. For example, $2p_z$ orbital of one atom can combine with $2p_z$ orbital of the other atom but not with the $2p_x$ or $2p_y$ orbitals because of different symmetries.
3. The combining atomic orbitals must overlap to the maximum extent. Greater the extent of overlap, the greater will be the electron density between the nuclei of a molecular orbital.

Types of Molecular Orbitals

- Molecular orbitals of diatomic molecules are titled as sigma (σ), pi (π), delta (δ) etc.
- In this nomenclature, the sigma molecular orbitals are symmetrical around the bond-axis while pi molecular orbitals are not symmetrical. For example, the linear combination of 1s orbitals centered on two nuclei produces two molecular orbitals which are symmetrical around the bond-axis.
- Such molecular orbitals are of the σ type and are designated as σ_{1s} and σ^*_{1s} .

- If internuclear axis is taken to be in the z-direction, it can be seen that a linear combination of $2p_z$ - orbitals of two atoms also produces two sigma molecular orbitals designated as $\sigma 2p_z$ and $\sigma^* 2p_z$.
- Molecular orbitals obtained from $2p_x$ and $2p_y$ orbitals are not symmetrical around the bond axis because of the presence of positive lobes above and negative lobes below the molecular plane.
- Such molecular orbitals are labeled as π and π^* . A π bonding MO has larger electron density above and below the inter-nuclear axis. The π^* anti-bonding MO has a node between the nuclei.

Energy level diagram for molecular orbitals

- 1s atomic orbitals on two atoms form two molecular orbitals designated as $\sigma 1s$ and $\sigma^* 1s$. In the same manner, the 2s and 2p atomic orbitals (eight atomic orbitals on two atoms) give rise to the following eight molecular orbitals:
- Antibonding MOs - $\sigma^* 2s$ $\sigma^* 2p_z$ $\pi^* 2p_x$ $\pi^* 2p_y$
- Bonding MOs - $\sigma 2s$ $\sigma 2p_z$ $\pi 2p_x$ $\pi 2p_y$

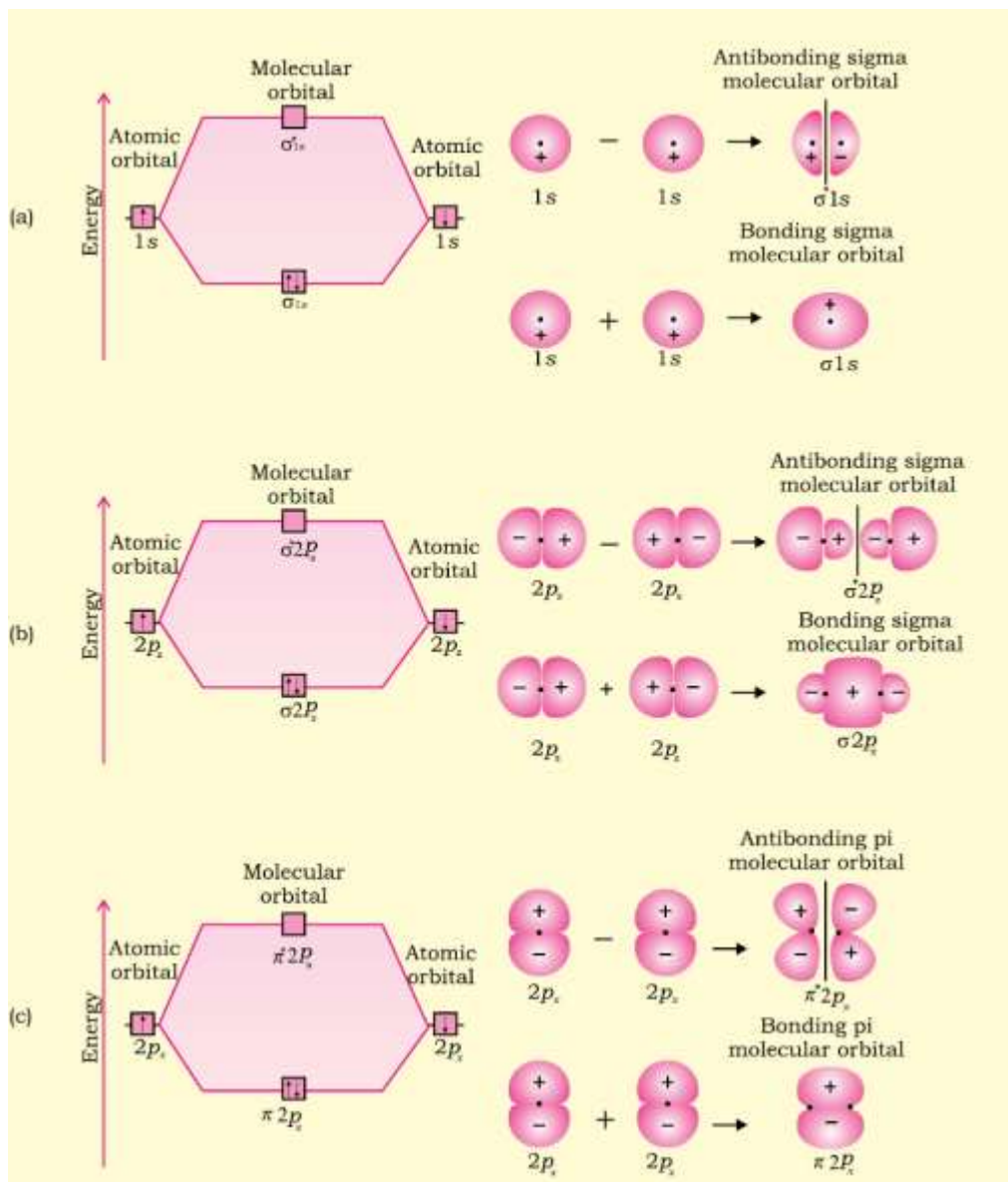


Figure: Contours and energies of bonding and anti-bonding molecular orbitals formed through combinations of (a) 1s atomic orbitals (b) $2p_z$ atomic orbitals and (c) $2p_x$ atomic orbitals.

- The increasing order of energies of various molecular orbitals for O_2 and F_2 is given below:
 $\sigma_{1s} < \sigma_{1s}^* < \sigma_{2s} < \sigma_{2s}^* < \sigma_{2p_z} < (\pi_{2p_x} = \pi_{2p_y}) < (\pi_{2p_x}^* = \pi_{2p_y}^*) < \sigma_{2p_z}^*$
- This sequence of energy levels of molecular orbitals is not correct for the remaining molecules $Li_2, Be_2, B_2, C_2, N_2$.

- It has been observed experimentally that for molecules such as B₂, C₂, N₂, etc. the increasing order of energies of various molecular orbitals is as follows:

$$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < (\pi 2p_x = \pi 2p_y) < \sigma 2p_z (\pi^* 2p_x = \pi^* 2p_y) < \sigma^* 2p_z$$
- The important characteristic feature of this order is that the energy of $\sigma 2p_z$ molecular orbital is higher than that of $\pi 2p_x$ and $\pi 2p_y$ molecular orbitals.

Electronic configuration and molecular behavior

- The distribution of electrons among various molecular orbitals is called the electronic configuration of the molecule. From the electronic configuration of the molecule, it is possible to get important information about the molecule as discussed below.
- **Stability of Molecules-** If N_b is the number of electrons occupying bonding orbitals and N_a the number occupying the anti-bonding orbitals, then:
 1. The molecule is stable if N_b is greater than N_a
 2. The molecule is unstable if N_b is less than N_a
- In case 1 more bonding orbitals are occupied and so the bonding influence is stronger and a stable molecule results. In case 2 the anti-bonding influence is stronger and therefore the molecule is unstable.
- **The order of the stability is O₂⁺ > O₂ > O₂⁻ > O₂²⁻ as the bond order of O₂⁺, O₂, O₂⁻, O₂²⁻ is 2, 2.5, 1.5 and 1 respectively.**
- **The order of the stability is N₂ > N₂⁺ > N₂⁻ > N₂²⁻ as the bond order of N₂, N₂⁺, N₂⁻, N₂²⁻ is 3, 2.5, 2.5 and 2 respectively.**

Bond order

- Bond order (b.o.) is described as one half the difference between the number of electrons present in the bonding and the anti-bonding orbitals.

$$\text{Bond order (b.o.)} = \frac{1}{2} (N_b - N_a)$$

- A positive bond order ($N_b > N_a$) means a stable molecule while a negative ($N_b < N_a$) or zero ($N_b = N_a$) bond order means an unstable molecule.

Nature of the bond

- Integral bond order values of 1, 2 or 3 correspond to single, double or triple bonds respectively as studied in the classical concept.

Bond-length

- The bond order between two atoms in a molecule may be taken as an approximate measure of the bond length.
- The bond length decreases as bond order increases.

Magnetic nature

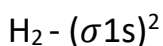
- If all the molecular orbitals in a molecule are doubly occupied, the substance is diamagnetic which means repelled by magnetic field.
- If one or more molecular orbitals are singly occupied it is paramagnetic (attracted by magnetic field) example - O_2 molecule.

BONDING IN SOME HOMONUCLEAR DIATOMIC MOLECULES

Bonding in some homo-nuclear diatomic molecules is as follows:

Hydrogen molecule (H_2)

- It is formed by the combination of two hydrogen atoms.
- Each hydrogen atom has one electron in 1s orbital. There are two electrons in hydrogen molecule which are present in σ_{1s} molecular orbital. So electronic configuration of H_2 molecule is



- The bond order of H_2 molecule can be calculated as given below:

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{2 - 0}{2} = 1$$

- This means that the two hydrogen atoms are bonded together by a single covalent bond.
- The bond dissociation energy of hydrogen molecule has been found to be 438 kJ mol^{-1} bond length equal to 74 pm. There is no unpaired electron is present in hydrogen molecule, so it is diamagnetic.

Helium molecule (He₂)

- The electronic configuration of helium atom is 1s².
- Each helium atom contains 2 electrons, so in He₂ molecule there would be 4 electrons. These electrons will be accommodated in $\sigma 1s$ and $\sigma^* 1s$ molecular orbitals leading to electronic configuration:
He₂ - $(\sigma 1s)^2 (\sigma^* 1s)^2$
- Bond order of He₂ = $\frac{1}{2} (2 - 2) = 0$
- He₂ molecule is therefore unstable and does not exist.
Similarly, it can be shown that Be₂ molecule $(\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2$ also does not exist.

Lithium molecule (Li₂)

- The electronic configuration of lithium is 1s², 2s¹. There are six electrons in Li₂. The electronic configuration of Li₂ =
Li₂ - $(\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2$
- The above configuration is also written as KK($\sigma 2s$)² where KK represents the closed K shell structure $(\sigma 1s)^2 (\sigma^* 1s)^2$.
- Bond order in Li₂ molecule is $\frac{1}{2} (4 - 2) = 1$.
- It means that Li₂ molecule is stable and since it has no unpaired electrons it should be diamagnetic. Indeed, diamagnetic Li₂ molecules are known to exist in the vapor phase.

Carbon molecule (C₂)

- The electronic configuration of carbon is 1s² 2s² 2p². There are twelve electrons in C₂. The electronic configuration of C₂ molecule is –
C₂ = $(\sigma 1s)^2 (\sigma^* 1s)^2 (\pi 2p_x)^2 = \pi 2p_y^2$ or
KK $(\sigma 2s)^2 (\sigma^* 2s)^2 (\pi 2p_x)^2 = \pi 2p_y^2$
- The bond order of C₂ molecule is $\frac{1}{2} (8 - 4) = 2$ and C₂ should be diamagnetic.
- It is important to note that double bond in C₂ consists of both π bonds because of the presence of four electrons in two π molecular orbitals. In most of the other molecules a double bond is made up of a σ -bond and a π -bond.

Oxygen molecule (O₂)

- The electronic configuration of oxygen atom - 1s² 2s² 2p⁴.
- Each oxygen atom has 8 electrons, In O₂ molecule there are 16 electrons. The electronic configuration of O₂ molecule =

$$O_2 = (\sigma_{1s})^2 (\sigma^*_{1s})^2 (\sigma_{2s})^2 (\sigma^*_{2s})^2 (\sigma_{2p_z})^2 (\pi_{2p_x})^2 (\pi_{2p_y})^2 (\pi^*_{2p_x})^1 (\pi^*_{2p_y})^1$$

$$O_2 = [KK (\sigma_{2s})^2 (\sigma^*_{2s})^2 (\sigma_{2p_z})^2 (\pi_{2p_x})^2 (\pi_{2p_y})^2, (\pi^*_{2p_x})^1 (\pi^*_{2p_y})^1]$$

- Bond order = $\frac{1}{2} [N_b - N_a] = \frac{1}{2} [10 - 6] = 2$
- O₂ molecule should be paramagnetic.

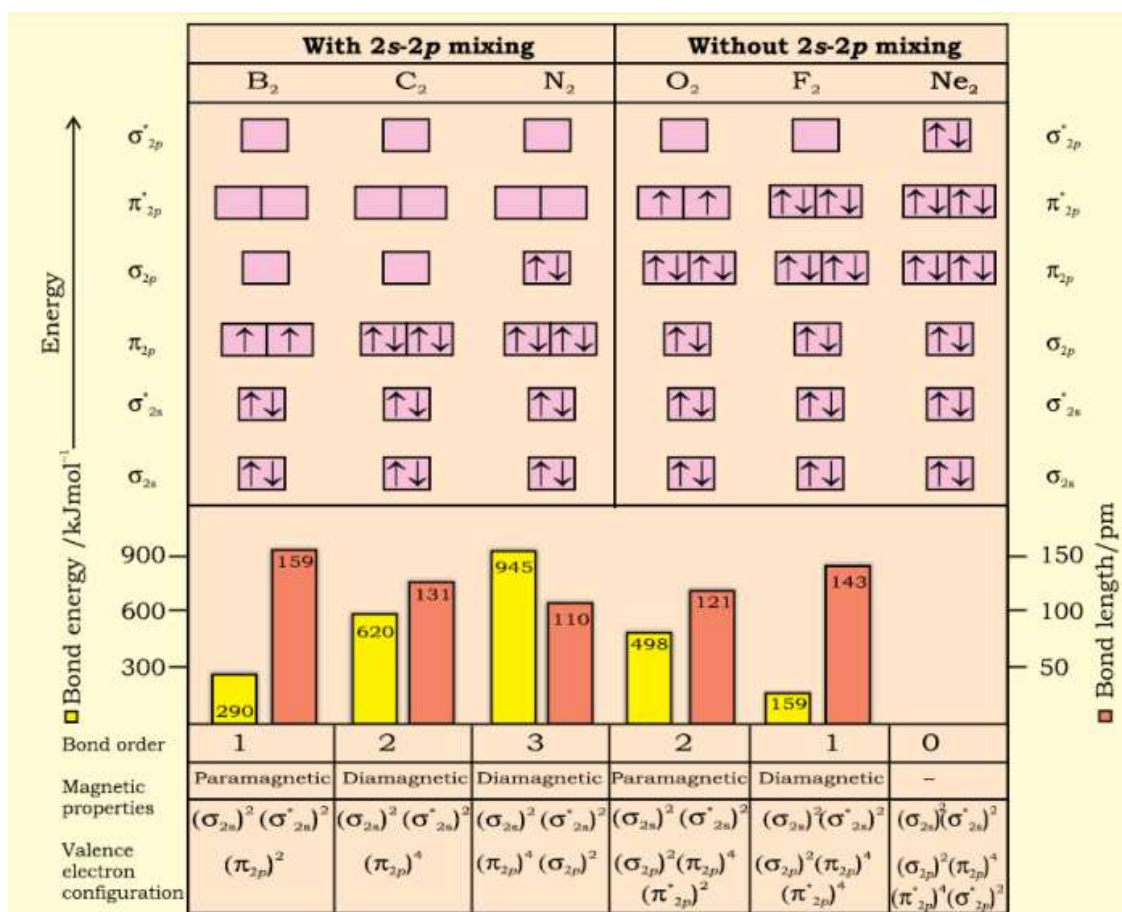
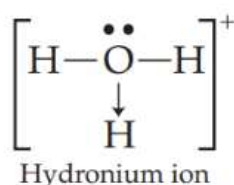
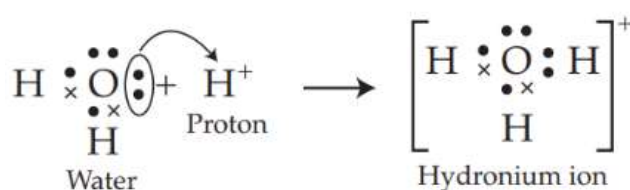


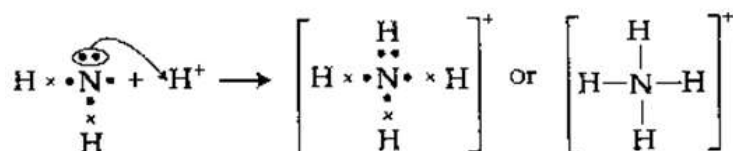
Figure: MO occupancy and molecular properties for B₂ through Ne₂

Co-ordinate (dative covalent) bonding

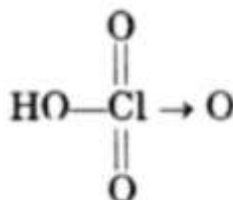
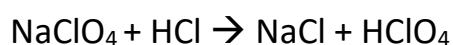
- A covalent bond is formed by sharing a pair of electrons by two atoms. The atoms are held together because electron pair is attracted by both of the nuclei.
- In the formation of a simple covalent bond, each atom supplies one electron to the bond. A co-ordinate bond also called a dative covalent bond; is a covalent bond in which both electrons come from the same atom.
- Formation of Hydronium ion



- Formation of ammonium ion

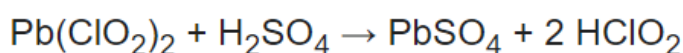
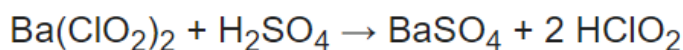


- Formation of Perchloric Acid

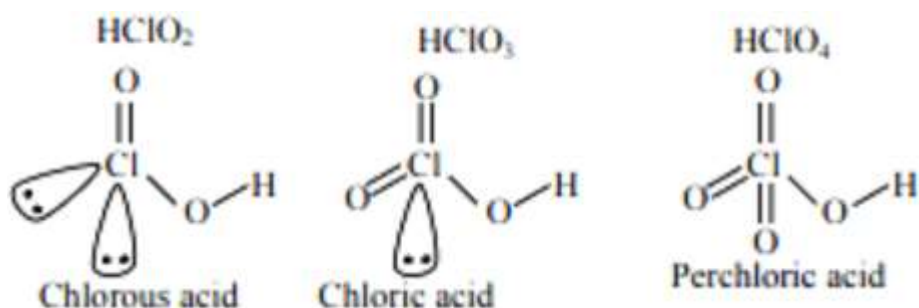
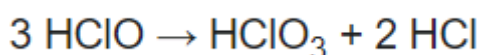
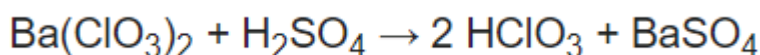


Perchloric acid

- Formation of Hypo Chlorous acid

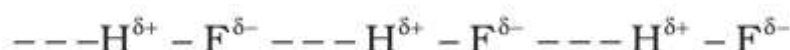


- Formation of Hypo Chloric Acid



HYDROGEN BONDING

- Nitrogen, oxygen and fluorine are the highly electronegative elements.
- When they are attached to a hydrogen atom to form covalent bond, the electrons of the covalent bond are shifted towards the more electronegative atom.
- This partially positively charged hydrogen atom forms a bond with the other more electronegative atom. This bond is known as H-bond and is weaker than the covalent bond.
- For example, in HF molecule, the H-bond exists between H-atom of one molecule and fluorine atom of another molecule as shown below—



- Hydrogen bond acts as a bridge between two atoms which holds one atom by covalent bond and other one by hydrogen bond.
- Hydrogen bond is represented by a dotted line (---) while a solid line represents the covalent bond.
- H-bond is the attractive force which binds hydrogen atom of one molecule with the electronegative atom (F, O or N) of another molecule.

Cause of formation of H-bond:

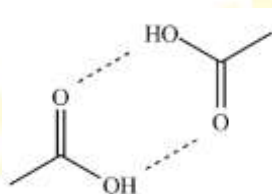
- When hydrogen is bonded to a strongly electronegative element **X**, the electron pair shared between the two atoms moves far away from hydrogen atom.
- As a result, the hydrogen atom becomes highly electropositive with respect to the other atom X.
- There is displacement of electrons towards X, so the hydrogen acquires fractional positive charge (δ^+) while X attains fractional negative charge (δ^-).
- This results in the formation of a polar molecule having electrostatic force of attraction which can be represented as follows:



Types of H-bonds

1. Intermolecular H-bond

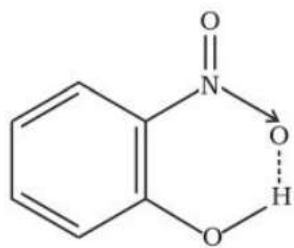
- It is formed between two different molecules of the same or different compounds. For example, H-bonding in the case of HF molecule, alcohol or water molecules.



Intermolecular H-bond in acetic acid

2. Intramolecular H-bond

- It is formed when hydrogen atom is in between the two highly electronegative (F, O, N) atoms present within the same molecule. For example, in o-nitrophenol the hydrogen is in between the two oxygen atoms.



Intramolecular hydrogen bonding in o-nitrophenol molecule

