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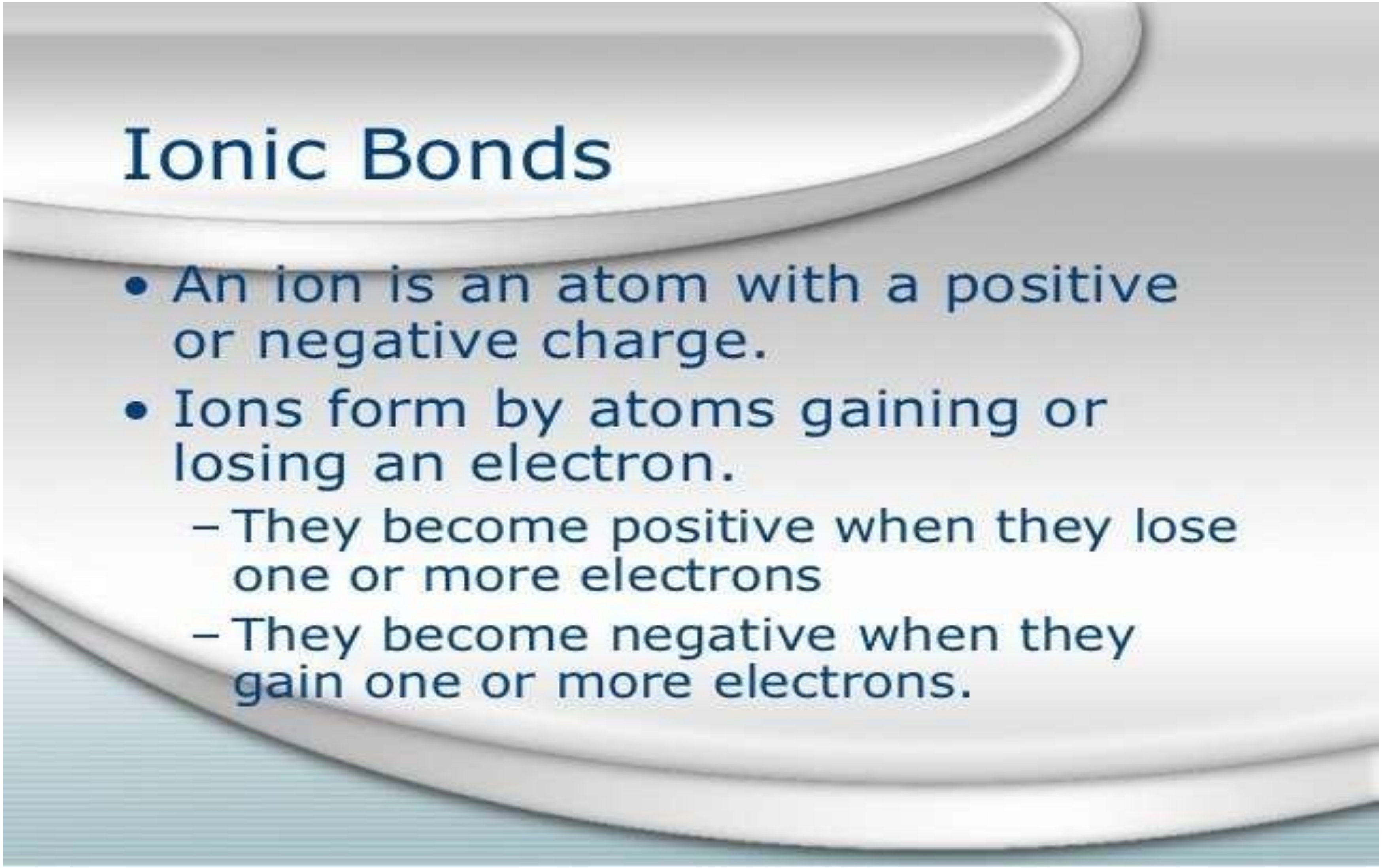
Bonding Models:

The ionic bond, Lattic energy, size effects, The covalent bond – preliminary approach, Valence Band Theory, Symmetry and overlap, Hybridization, Delocalization, Experimental measurement of charge distribution in Molecules

Ionic Bond


Ionic Bonds
• An ion is an atom with a positive or negative charge.
• Ions form by atoms gaining or losing an electron.
– They become positive when they lose one or more electrons
– They become negative when they gain one or more electrons.

Ionic Bonds

- Ionic bonds occur between metals and non metals.
  - Metals form positive ions
  - Nonmetals form negative ions.

Ionic Bonds

- Positive ions are called ***cations***
- Negative ions are called ***anions***

- ***Cations*** have lost electrons and ***anions*** have gained electrons.

Ionic Bonds

- Because opposites attract, when ions form, they bond to one another due to magnetic attraction.
  - EX: Na (sodium) needs to lose one electron to become stable, Cl (chlorine) needs to gain one electron to become stable. Na becomes positive, Cl becomes negative and they bond due to their opposite charges.

Lattice energy: The energy of crystal lattice of an ionic compound is the energy released when ions come together to form a crystal.

Lattice Energy

- The extra stability that accompanies the formation of the crystal lattice is measured as the **lattice energy**
- The lattice energy is the energy released when the solid crystal forms from separate ions in the gas state
- Always exothermic
- Hard to measure directly, but can be calculated from knowledge of other processes
- Lattice energy $\propto$ charge $\propto$ 1/ distance b/w ions

Where can lattice energy be valid?

Lattice energies are associated with many interactions, as cations and anions pack together in an extended lattice.

For **covalent bonds**, the bond dissociation energy is associated with the interaction of just two atoms.

Covalent Compounds ✗

Ionic Compounds ✓

Metallic Compounds??

Introduction to Covalent Bonding

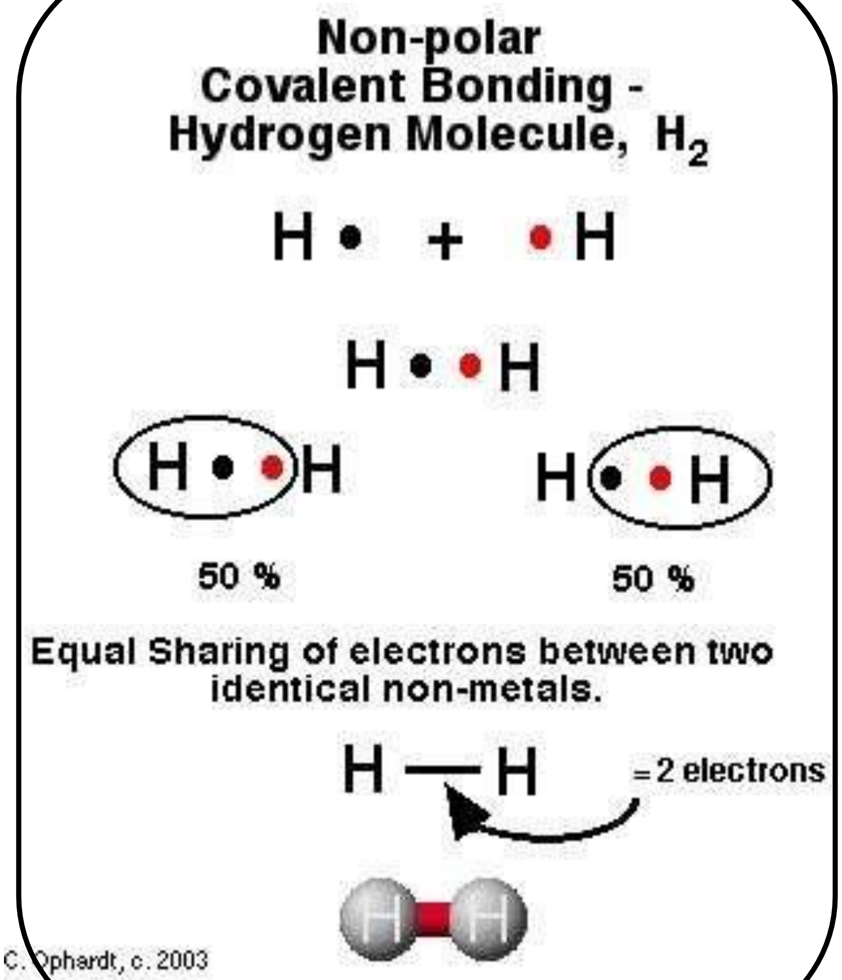
Introduction to Covalent Bonding: In the formation of covalent bond two nonmetals can share an electrons to form covalent bond.

There are two forms of covalent bonding:

1. **Non-polar bonding** with an equal sharing of electrons e.g. H_2

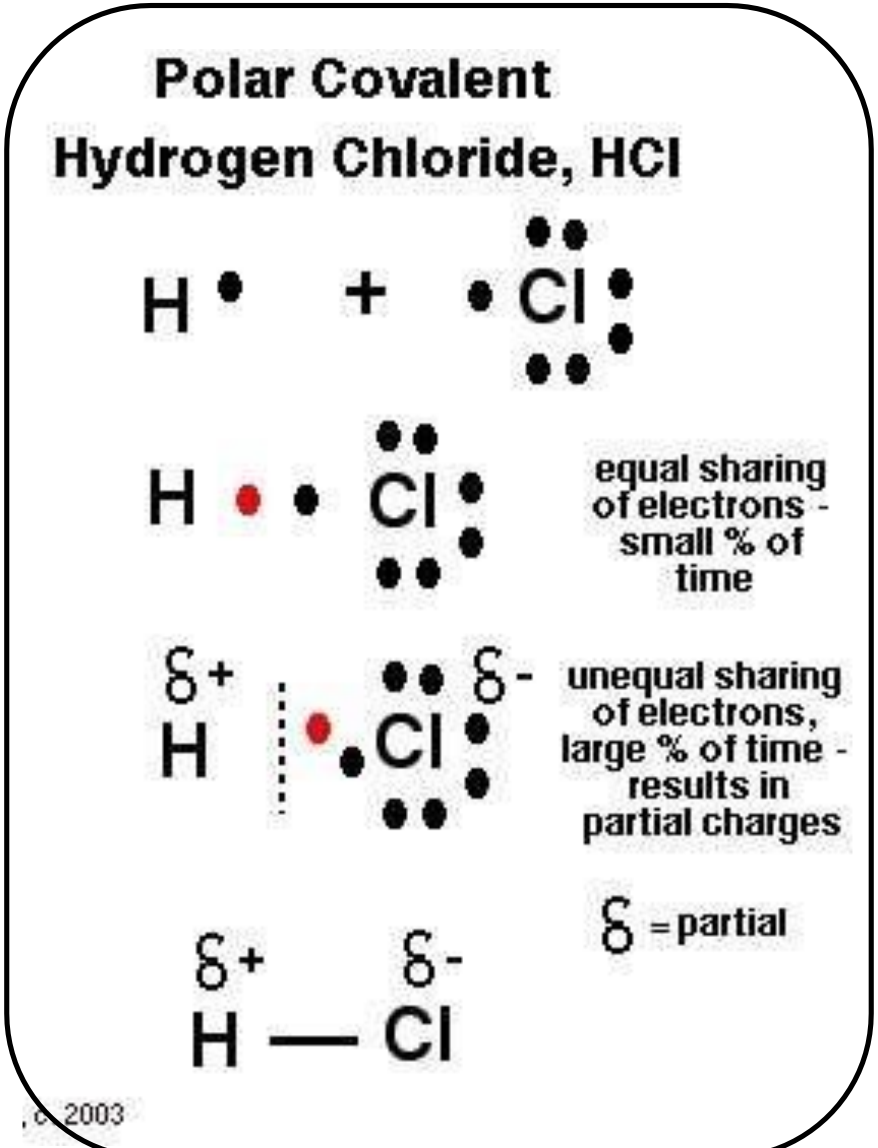
2. **Polar bonding** with an unequal sharing of electrons. The number of shared electrons depends on the number of electrons needed to complete the octet e.g. HCl

NON-POLAR BONDING results when two **identical non-metals equally share** electrons between them.



The simplest non-polar covalent molecule is hydrogen. Each hydrogen atom has one electron and needs two to complete its first energy level. Since both hydrogen atoms are identical, neither atom will be able to dominate in the control of the electrons. The electrons are therefore shared equally.

POLAR BONDING results when two **different non-metals unequally share** electrons between them.



Hydrogen Chloride forms a polar covalent molecule. Hydrogen has one electron in its outer energy shell. Since 8 electrons are needed for an octet, they share the electrons. **Chlorine has tendency to o keep its own electron and also draw away the other atom's electron.** As a result, the chlorine acquires a "partial" negative charge. At the same time, since hydrogen loses the electron most - but not all of the time, it acquires a "partial positive" charge.

Types of Covalent Bonding

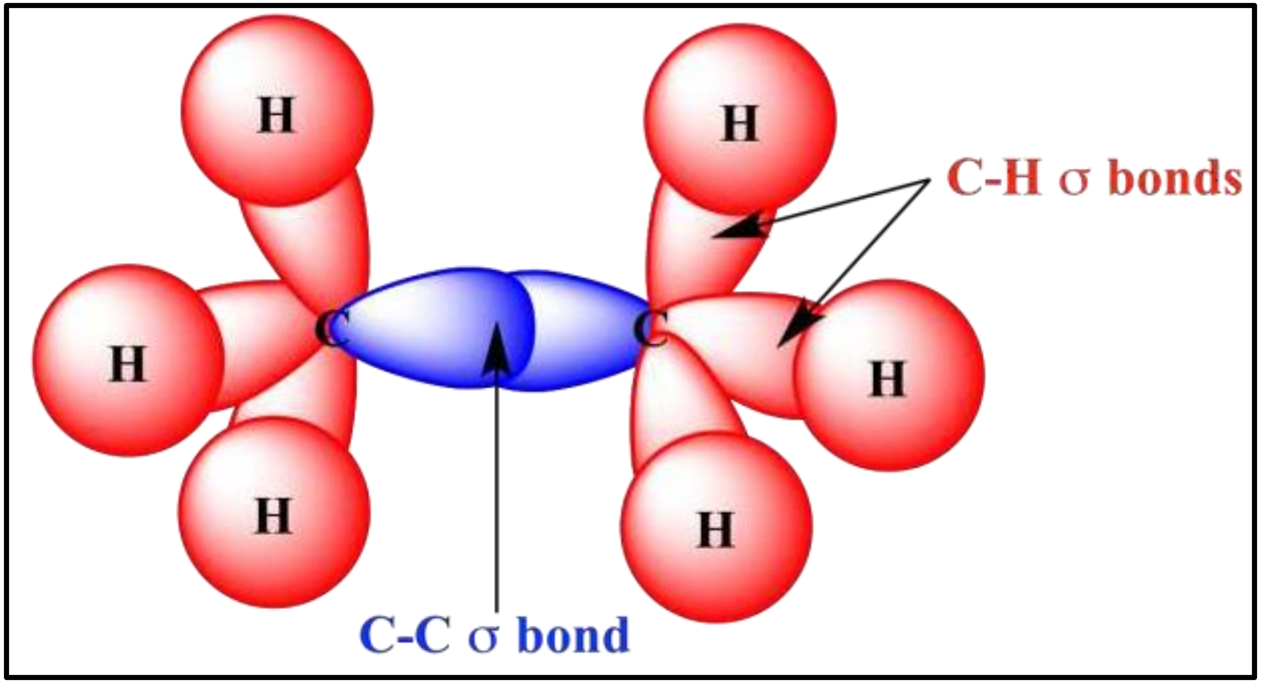
Types of covalent bonding

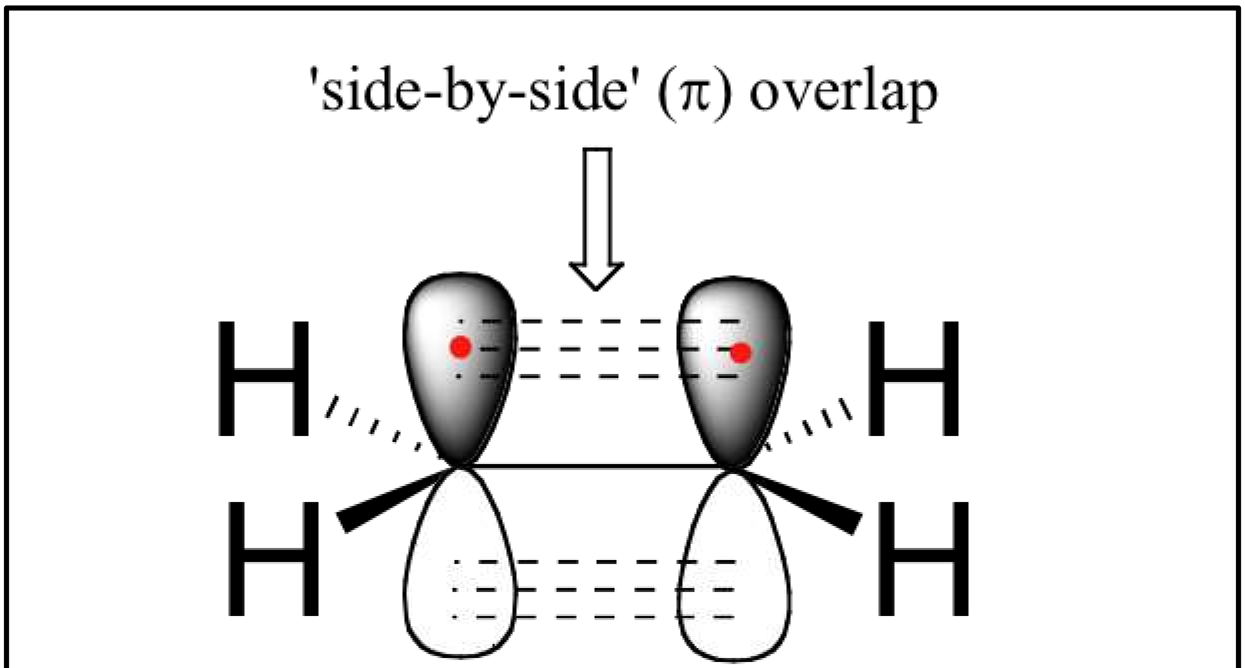
1) **Sigma bond**
2) **Pi- Bond**

Atomic orbitals (except for s orbitals) have specific directional properties leading to different types of covalent bonds.

Sigma (σ) bonds are the strongest covalent bonds and are due to head-on overlapping of orbitals on two different atoms. A single bond is usually a σ bond.

Pi (π) bonds are weaker and are due to lateral overlap between p (or d) orbitals. A double bond between two given atoms consists of one σ and one π bond, and a triple bond is one σ and two π bonds


H
H
C-H σ bonds
H
C
C
H
H
H
C-C σ bond


'side-by-side' (π) overlap
H
H
H
H

Valence Bond Theory(VBT)

Valence Bond Theory (VBT): In order to explain the covalent bonding , Heitler and London developed the VBT.

Postulates of VBT:

i. A covalent bond is formed when half filled valence orbital of an atom overlaps with half filled valence orbital of another atom.

ii. The electrons in the half filled valence orbital must have opposite spin.

iii. During bond formation the half filled orbitals overlap and the opposite spins of electron get neutralized. So the increased electron density decreases the nuclear repulsion and energy is released during overlapping the orbitals.

iv. Greater the extent of overlap stronger will be the bond formed.

Valence Bond Theory(VBT)

v. If an atom possess more than one unpaired electrons, it can form more than one bond. So the number of bonds formed will be equal to number of half filled orbitals in the valance shell.

vi. The distance at which attractive and repulsive force balance each other is the equilibrium distance. At this distance the total energy of bonded atoms minimum and stability is maximum.

vii. The electrons paired in the valance shell can not participated in the bond formation.

viii. During bond formation S orbital can overlap in any direction (spherical). The p orbital can overlap only in x, y, z direction. (d and f also). So covalent bond is directional.

Overlap and Symmetry of atomic orbitals

- ❖ Formation of bond has been explained on the basis of overlap of atomic orbitals having same energy and symmetry.
- ❖ The strength of a bond depends upon the extent of overlap of atomic orbitals. So, greater the overlap stronger the bond.
- ❖ The orbitals holding the electrons vary in shape, energy, symmetry and size. So the extent of overlap depends upon shape and size of orbital.

- **Types of bond:** Sigma bond (σ bond): Overlap along the axis
- Pi bond (π bond): lateral overlapping

Overlap and Symmetry of atomic orbitals

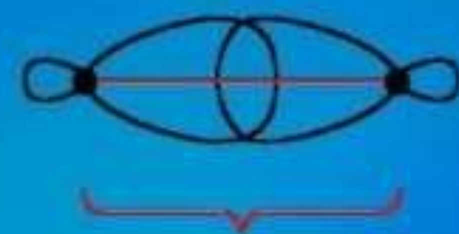
Valence Bond Theory

iTutor

There are two types of covalent bonds based on the pattern of overlapping as follows:

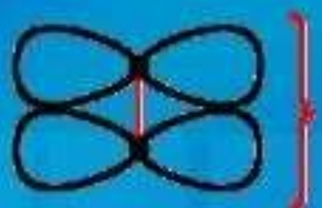
σ-bond

A sigma bond (symbol: σ) is a covalent bond formed via linear overlap of two orbital's.



σ bond

π-bond



Π bond

A pi bond (symbol: π) is a covalent bond formed via parallel overlap of two orbital's.

Overlap and Symmetry of atomic orbitals

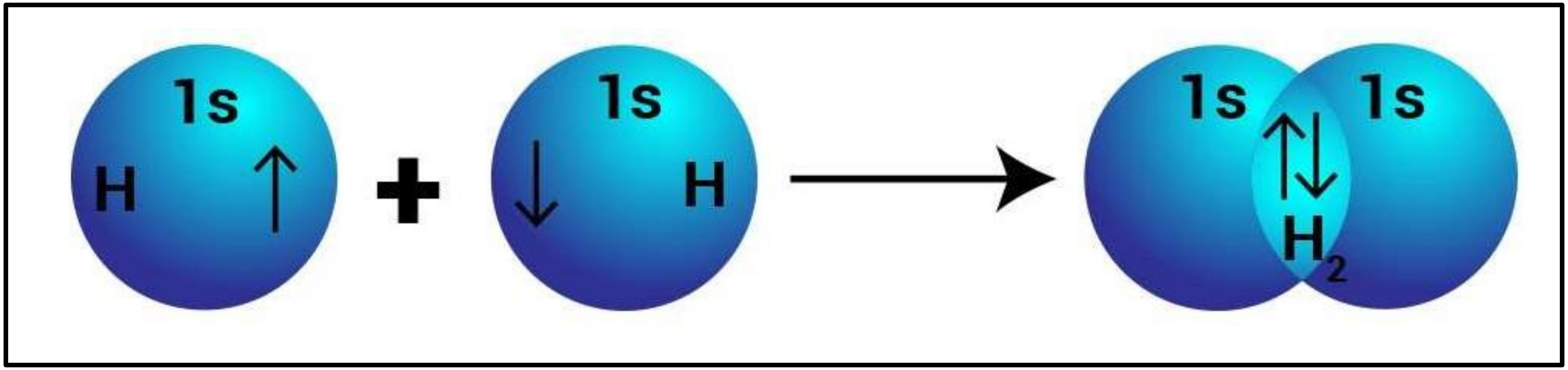
σ-bond

- The covalent bond formed due to overlapping of atomic orbital along the inter nucleus axis is called σ-bond. It is a stronger bond and cylindrically symmetrical.
- Depending on the types of orbital's overlapping, the σ-bond is divided into following types:

(i): $\sigma_{s\text{-}s}$ bond, (ii): $\sigma_{p\text{-}p}$ bond, (iii): $\sigma_{s\text{-}p}$ bond:

σ s-s overlap

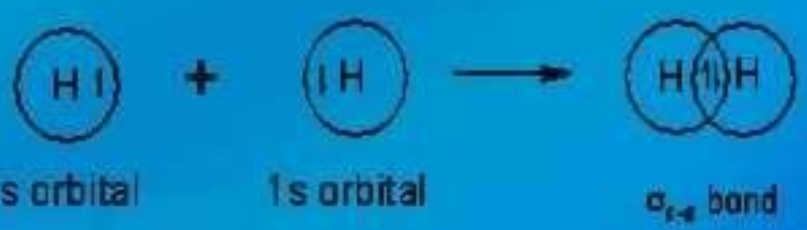
The 1s orbital of two hydrogen atoms overlap along internuclear axis to form σ bond between the atoms in H_2 molecules.



σ s-s overlap

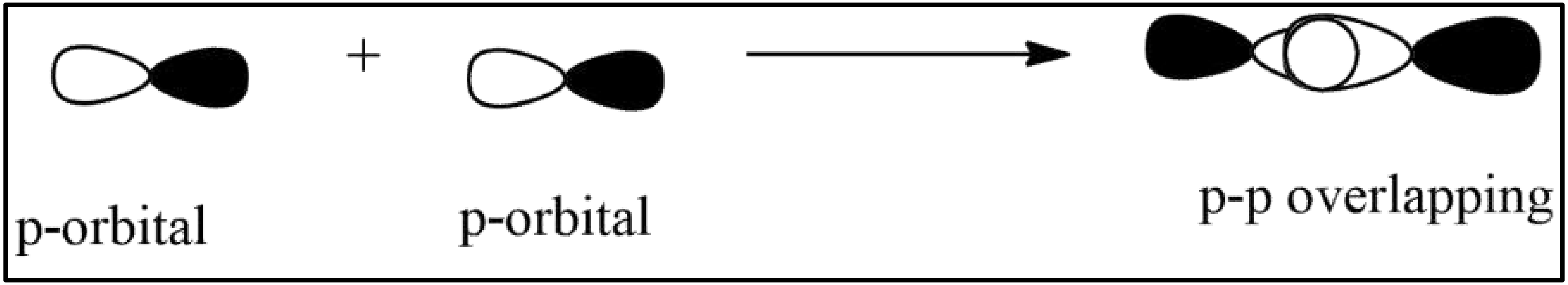
H2 molecule

- The electronic configuration of hydrogen atom in the ground state is $1s^1$.
- In the formation of hydrogen molecule, two half filled 1s orbital's of hydrogen atoms overlap along the inter-nuclear axis and thus by forming a $\sigma_{s\text{-}s}$ bond.



σ p-p overlap

This type of overlap takes place when two p orbitals from different atoms overlap along internuclear axis. Eg. F_2 molecule, Cl_2 molecule



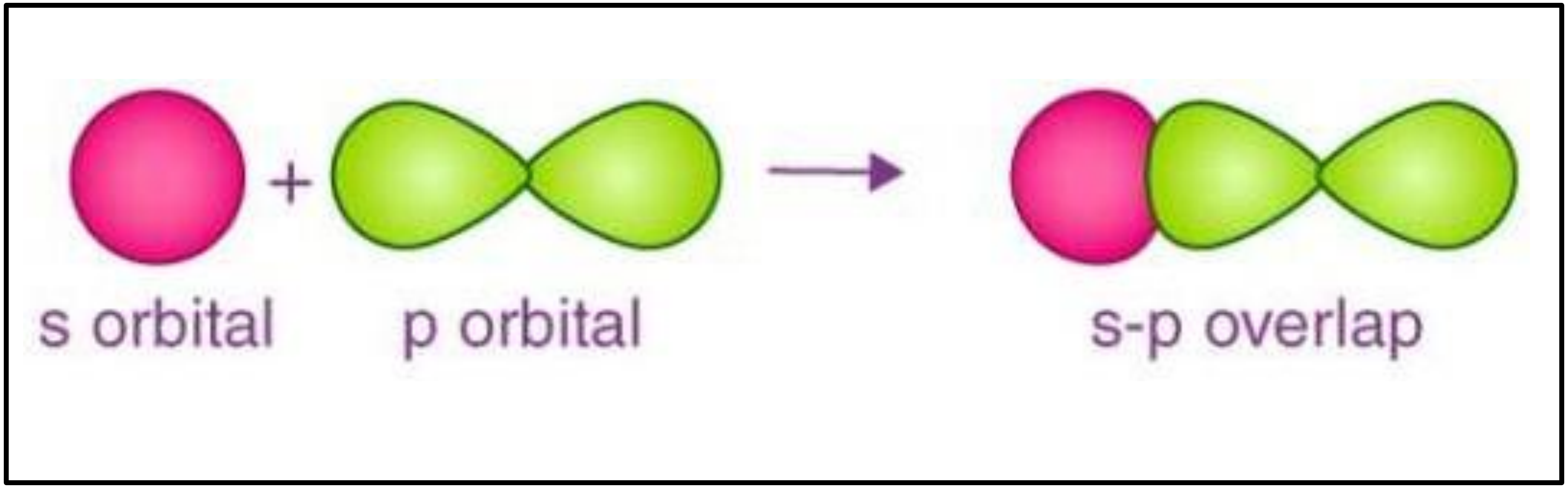
σ p-p overlap

Cl2 molecule

- The electronic configuration of Cl atom in the ground state is [Ne]$3s^2\ 3p_x^{\ 2}\ 3p_y^{\ 2}\ 3p_z^{\ 1}$.
- The two half filled $3p_z$ atomic orbital's of two chlorine atoms overlap along the inter-nuclear axis and thus by forming a $\sigma_{p\text{-}p}$ bond.

σ s-p overlap

In this type of overlap one half filled s orbital and one half filled p orbital of another atom overlap along the internuclear axis. Eg. HF molecule.



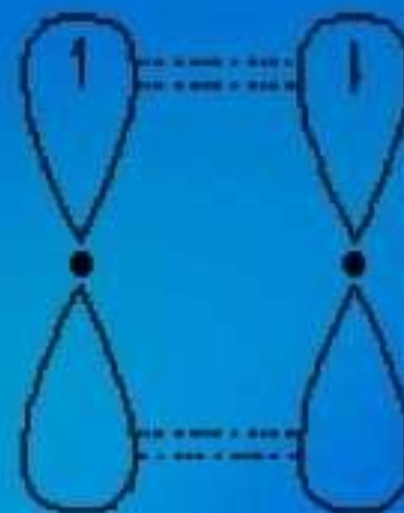
σ s-p overlap

HCl molecule

- In the ground state, the electronic configuration of hydrogen atom is $1s^1$.
- And the ground state electronic configuration of Cl atom is $[Ne]3s^2\ 3p_x^2\ 3p_y^2\ 3p_z^1$.
- The half filled 1s orbital of hydrogen overlap with the half filled $3p_z$ atomic orbital of chlorine atom along the inter-nuclear axis to form a σ_{s-p} bond.

π-bond

- The covalent bond formed by sidewise overlapping of atomic orbital's is called π- bond. In this bond, the electron density is present above and below the inter nuclear axis. It is relatively a weaker bond since the electrons are not strongly attracted by the nuclei of bonding atoms.

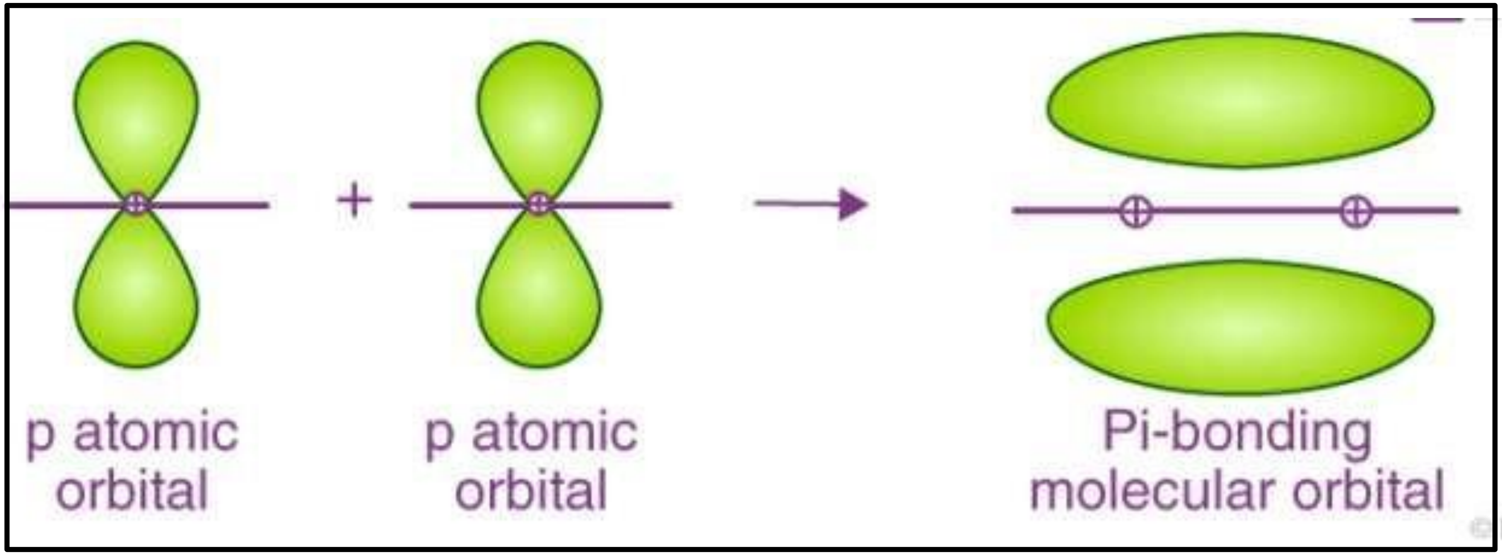


π_{p-p} bond

Note: The 's' orbital's can only form σ-bonds, whereas the p, d & f orbital's can form both σ and π-bonds.

π p-p overlap

When two half filled orbitals of two atoms overlap sideways (lateral) it is called π overlap and it is perpendicular to internuclear axis. Eg N2, O2 molecule.



π p-p overlap

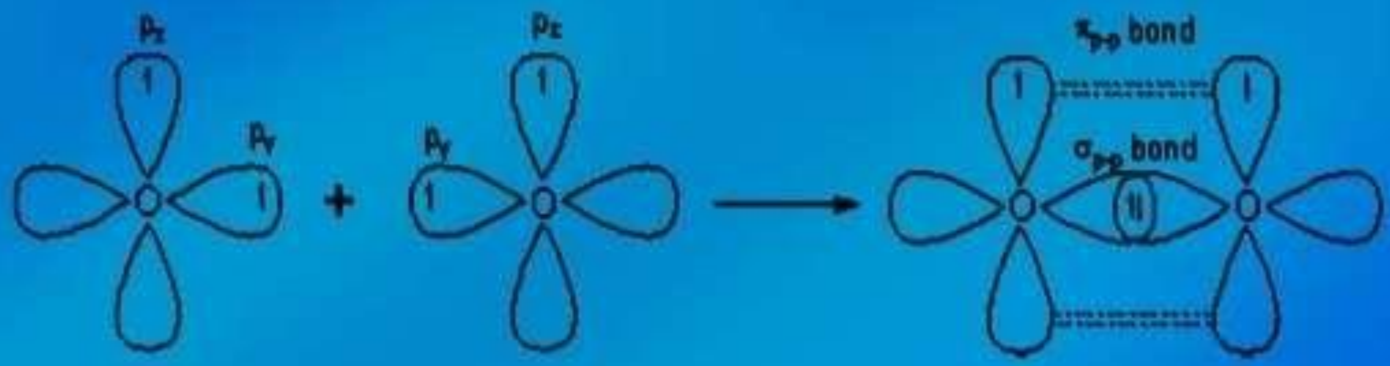
O2 molecule

- The electronic configuration of O in the ground state is [He] $2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$.
- The half filled $2p_y$ orbital's of two oxygen atoms overlap along the inter-nuclear axis and form $\sigma_{p\text{-}p}$ bond.
- The remaining half filled $2p_z$ orbital's overlap laterally to form a $\pi_{p\text{-}p}$ bond.

π p-p overlap

O2 molecule

- Thus a double bond (one $\sigma_{p\text{-}p}$ and one $\pi_{p\text{-}p}$) is formed between two oxygen atoms.



π p-p overlap

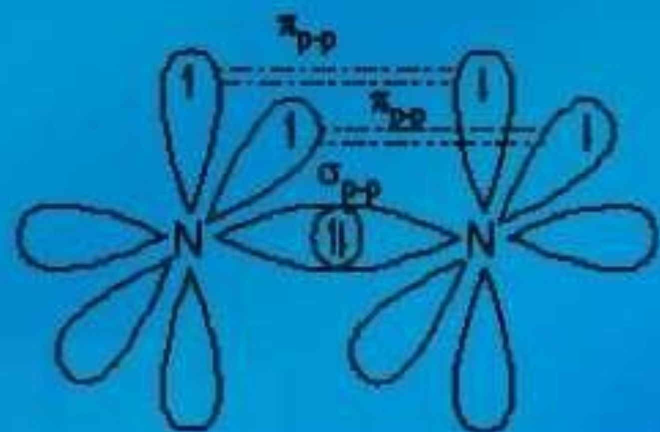
N2 molecule

- The ground state electronic configuration of N is [He] $2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^1$.
- A $\sigma_{p\text{-}p}$ bond is formed between two nitrogen atoms due to overlapping of half filled $2p_x$ atomic orbital's along the inter-nuclear axis.

π p-p overlap

N2 molecule

- The remaining half filled $2p_y$ and $2p_z$ orbital's form two $\pi_{p\text{-}p}$ bonds due to lateral overlapping. Thus a triple bond (one and two) is formed between two nitrogen atoms.



Thank You!