ATOMIC ORBITAL THEORY OF COVALENT BOND

According to orbital concept, a covalent bond is formed by the overlapping of atomic orbitals. This overlapping can take place either along the axes of orbitals or perpendicular to their axes. Thus, it gives rise to two types of bond σ and π bonds.

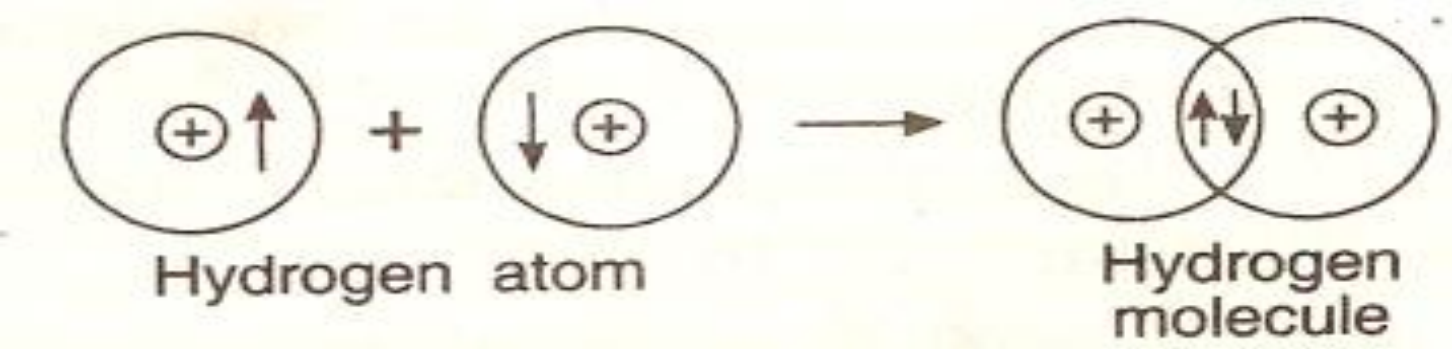
1. **Sigma bond** (σ): The σ bond formed as a result of end to end overlapping, *i.e.,* the electron density is concentrated in between the two atoms and a line joining the two atoms. σ bond is very strong due to the maximum overlapping in the σ bond. The overlapping may be of 3 types :

(i) *s-s* overlapping (ii) *s-p* overlapping (iii) *p-p* overlapping.

ATOMIC ORBITAL THEORY OF COVALENT BOND

(i) **s-s overlapping:** Since the *s* orbital is spherically symmetrical, so due to its overlapping with another *s*-orbital the maximum overlapping take place.

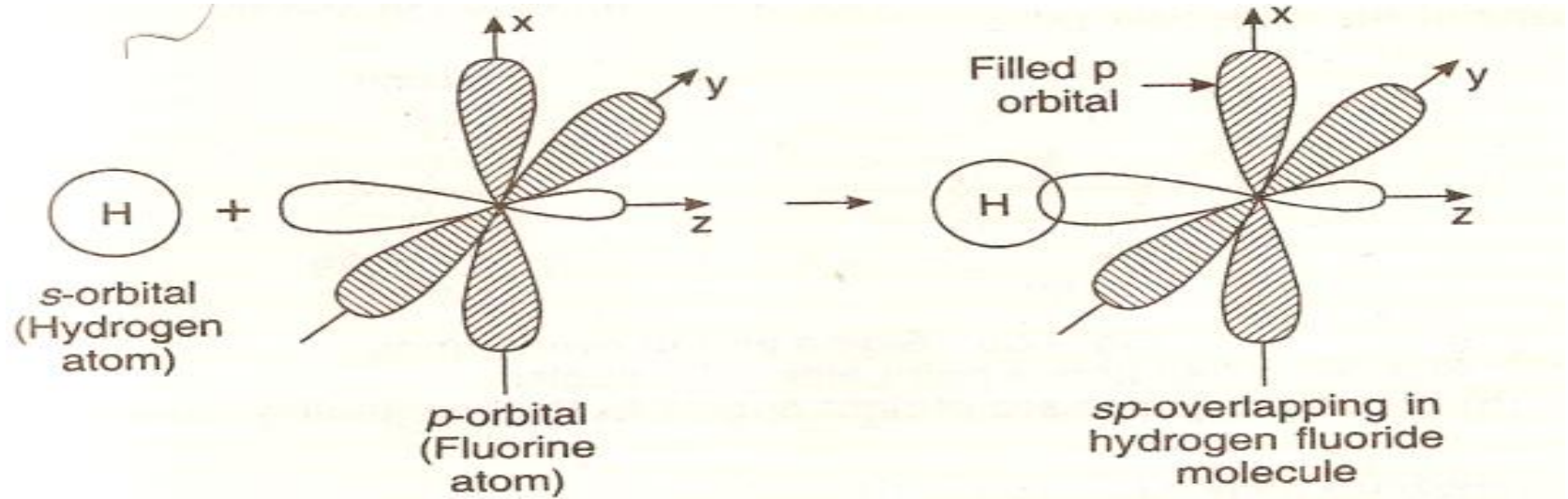
Example: Hydrogen atom ($1s^1$) has a single electron. When their s orbital overlap with each other form a covalent bond, this type of overlapping is called s-s overlapping**.**



ATOMIC ORBITAL THEORY OF COVALENT BOND

(ii) s-p overlapping: Formation of σ bond as a resuslt of *s*-p overlapping is illustrated by the formation of halogen acids like hydrogen fluoride molecule, and hydrogen chloride molecule .

Example: The outer electronic configuration of fluorine atom is $2s^2p^5$. It needs one electron more in its outer shell to acquire the stable s^2p^6 configuration and this type of overlapping is called s-p overlapping.

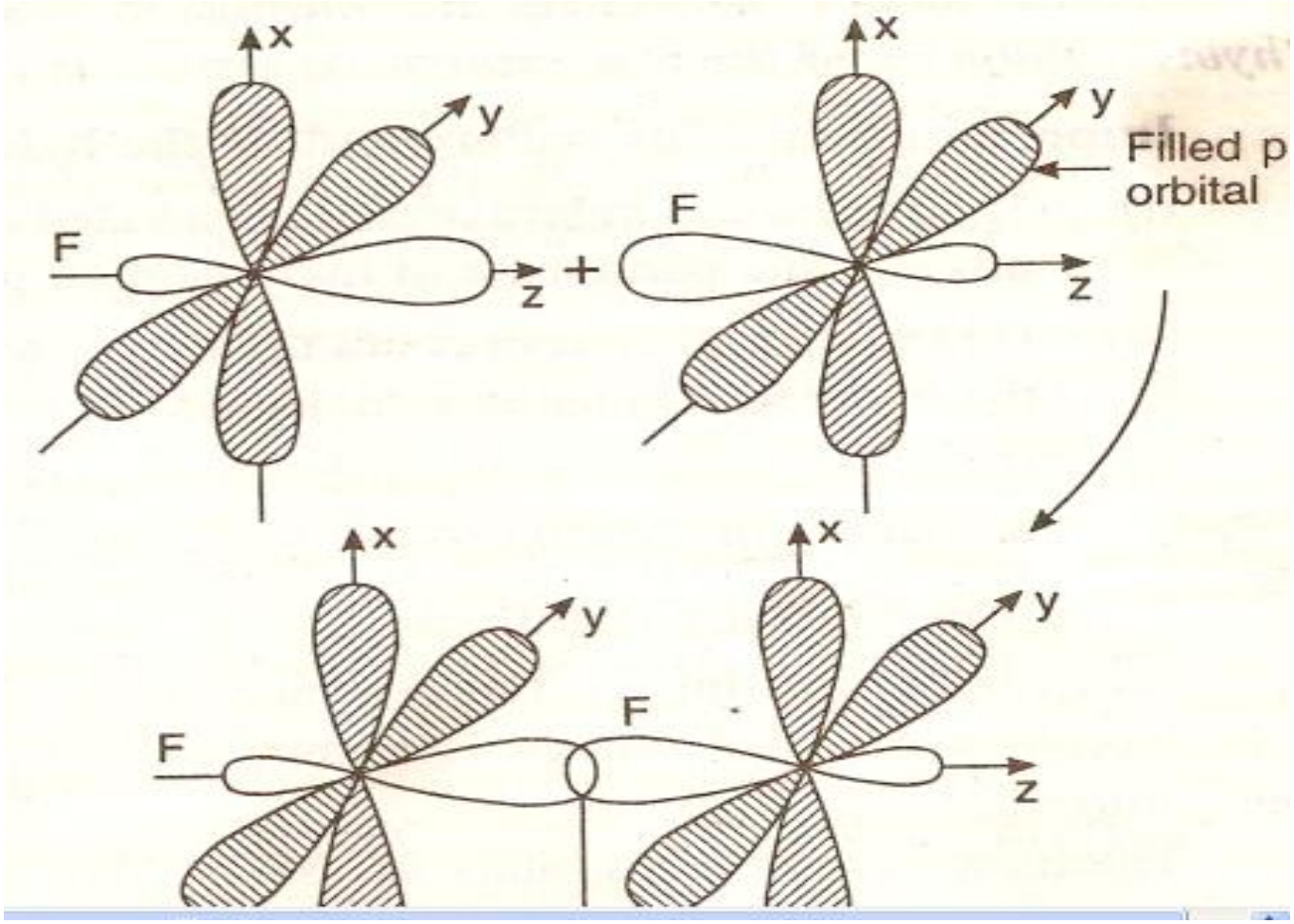


ATOMIC ORBITAL THEORY OF COVALENT BOND

(iii) p-p overlapping: Formation of σ bond as a result of axial overlapping of *p-p* orbitals is illustrated by the formation of halogen molecules (fluorine or chlorine).

Example : In the formation of fluorine molecule the half filled p-orbital of one atom overlaps with a similar p-orbitals of another atom to form F_2 molecule. This type of overlapping is called p-p overlapping.

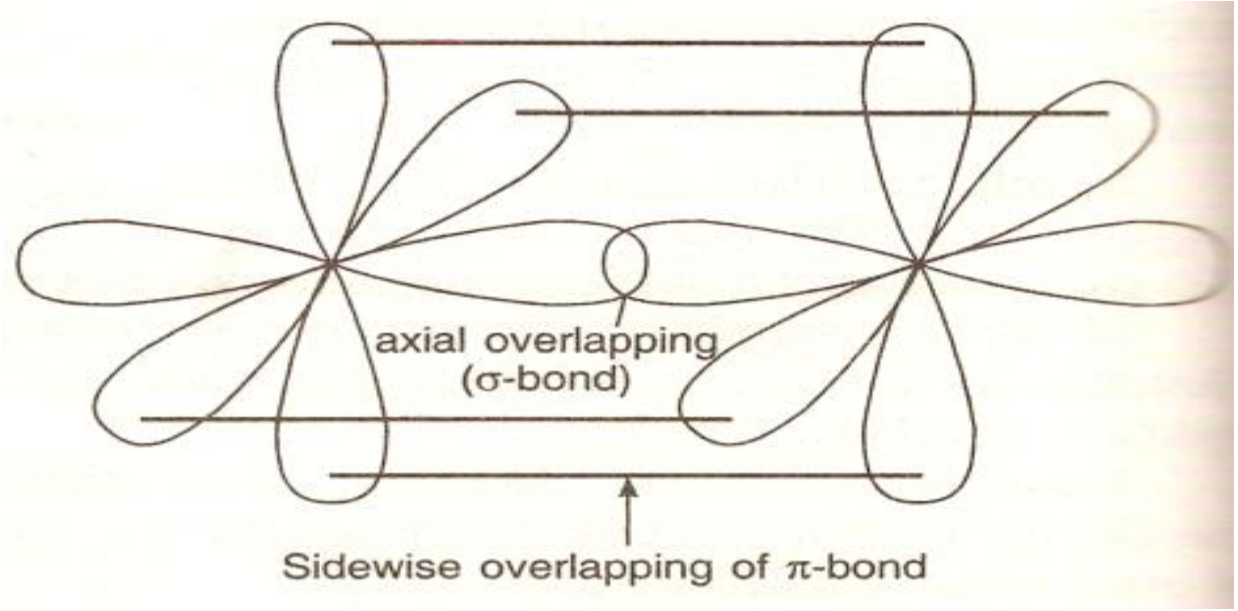
ATOMIC ORBITAL THEORY OF COVALENT BOND



ATOMIC ORBITAL THEORY OF COVALENT BOND

(2) Pi (π) bond: . The bond formed as a result of sideways overlapping of *p*-*p* orbitals is known as a π bond. In this case the electron density also concentrates between the atoms, but on either side of the line joining the atoms.

Example: Formation of Pi bond in N_2 Molecule.



HYBRIDIZATION

Definition: The phenomenon of mixing up of atomic orbitals of similar energies and formation of equivalent number of entirely new orbitals of identical shape and energy is known as "hybridization" and the new orbitals so formed is called as "hybrid orbitals".

Important points for understanding the hybridization:

(i) The number of hybrid orbitals generated is equal to the number of pure atomic orbitals that participate in hybridization process.

(ii) Hybridization concept is not applicable to isolated atoms. It is used to explain the bonding scheme in a molecule.

(iii) Covalent bonds is polyatomic molecules are formed by the overlap of hybrid orbitals or of hybrid orbitals with unhybridized ones.

HYBRIDIZATION

Types of Hybridization

(1) sp-hybridization: The combination of one s and one p-orbitals to form two hybrid orbitals of equal energy is known as sp-hybridization.

Example: In BeF_2 Molecule the sp-hybridized orbitals of Be overlap with the half-filled orbitals of two fluorine atoms to give a **linear shape.**

HYBRIDIZATION

Structure of BeF_2 Molecule