Organic Chemistry 101 C

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Atomic orbitals

Atomic orbitals are the regions of space in which electrons are usually to be found.

There are a large number and various shapes of atomic orbitals.

The shapes of atomic orbitals and the orientation define the probability of finding the electron along some certain directions

Each of the orbital is denoted by
a number (1, 2. 3,…)
and
a letter (s, p, d, ..).

The number is denoted to the energy level of the electron

The number 1 refers to the energy level that is closest to the nucleus, however, 2 refers to the next level of energy further out.

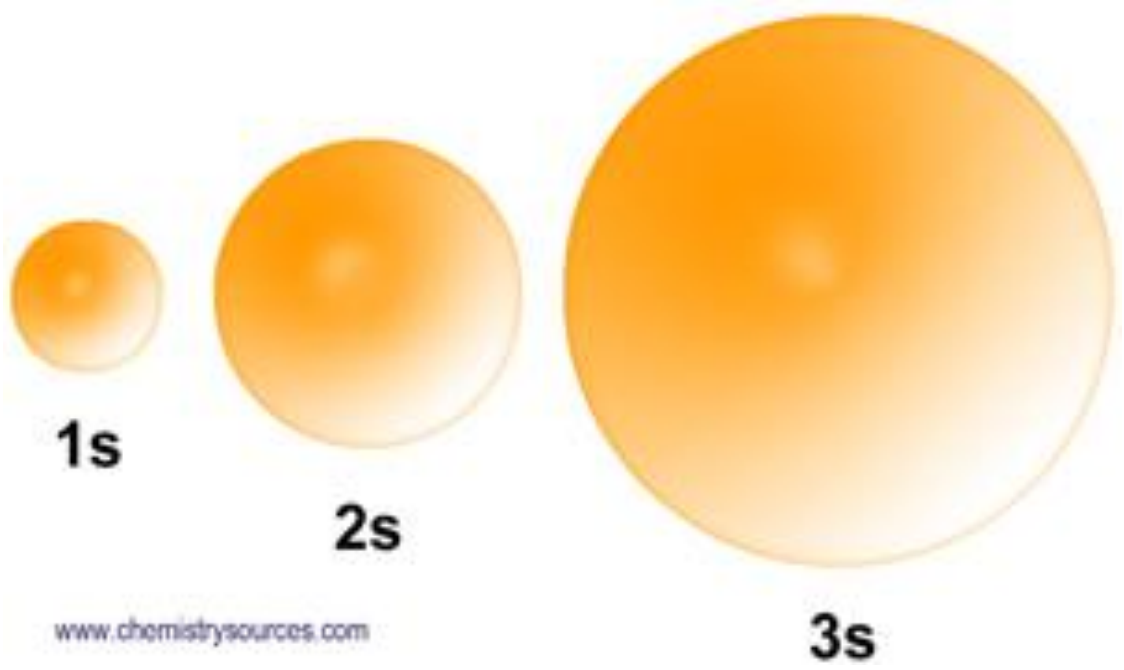
The symbols s, p, d, f originally comes from the words meaning sharp, principal, diffuse and fundamental respectively. This has been used to ascertain the spectral lines in the atomic spectra of different atoms

S orbital

S orbital is spherical in shape

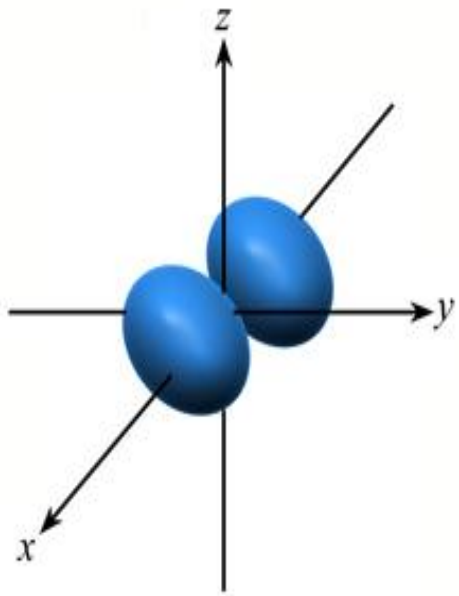
i.e., in an *s* orbital the electron distribution is symmetrical around the nucleus in all directions.

However the size of *s* orbital depends on principal quantum number. Large n means large size. Thus 3*s* orbital is larger than 2sorbital.

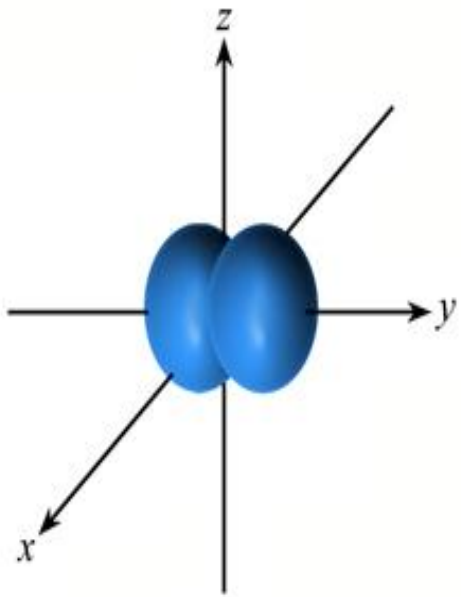


p orbitals

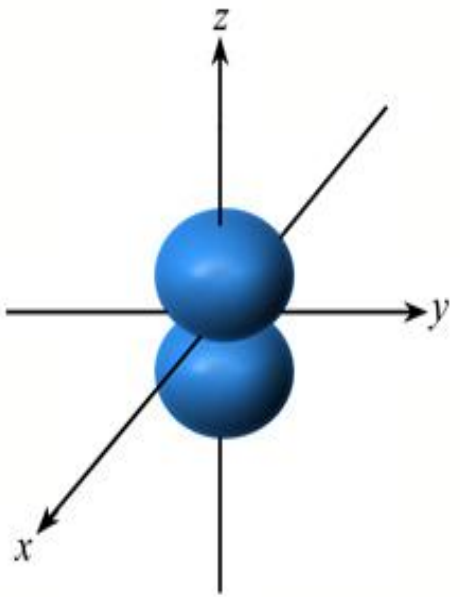
There are three *p* orbitals (p_x, p_y, p_z) as the values of m are three i.e., -1, 0, +1 and all are of equal energy. They are dumb-bell shaped and oriented along three axis x, y and z respectively.



$2p_x$



$2p_y$



$2p_z$

Molecular orbitals

Atoms combine together to lower down the energy of the system to attain stability.

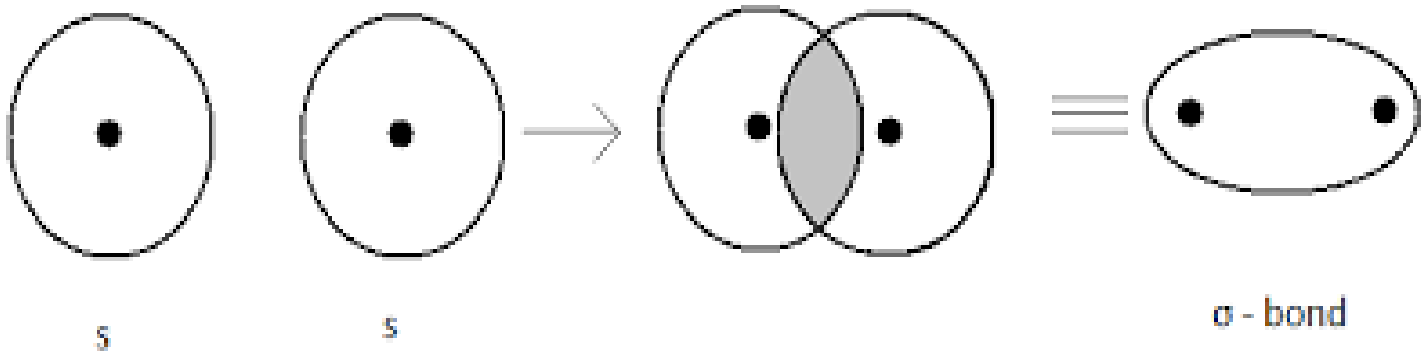
For example, hydrogen prefers to exist as H_2 molecule instead of isolated hydrogen atom because H_2 requires lesser energy than isolated H atom.

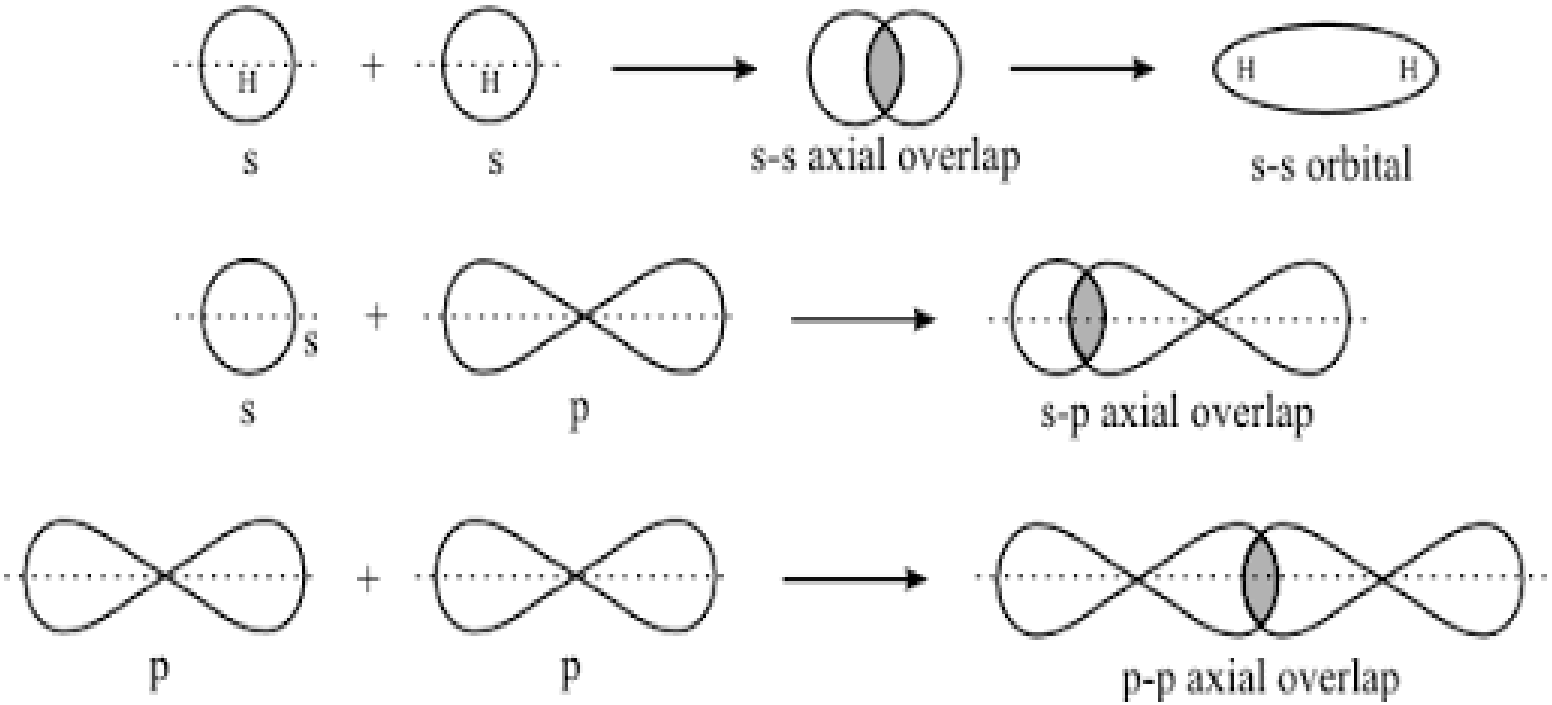
The atomic orbitals overlap together to form molecular orbitals of the molecules.

This overlap of atomic orbitals can obtain by two ways

Collinear overlaps

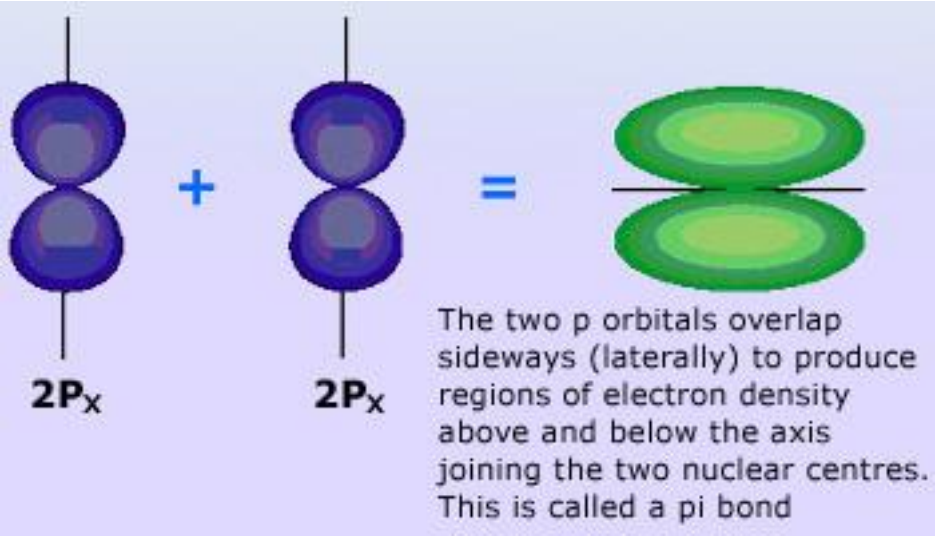
Overlap along the axis of the nuclei to form sigma bonds (σ bonds).




H
H
s
s
s-s axial overlap
H
H
s-s orbital
s
s
p
s-p axial overlap
p
p
p-p axial overlap

Collateral overlap

Overlapping of the parallel atomic orbitals laterally to form bi bonds (π bonds) .



σ bonds are formed from collinear overlaps, while π bonds are formed from collateral overlaps