University of Thi-Qar …
College Of Science ……….. Department of Chemistry

Organic Chemistry
Second Stage

Lecture 1 (Bonding and structure)

Dr.Athraa Hameed Mekky

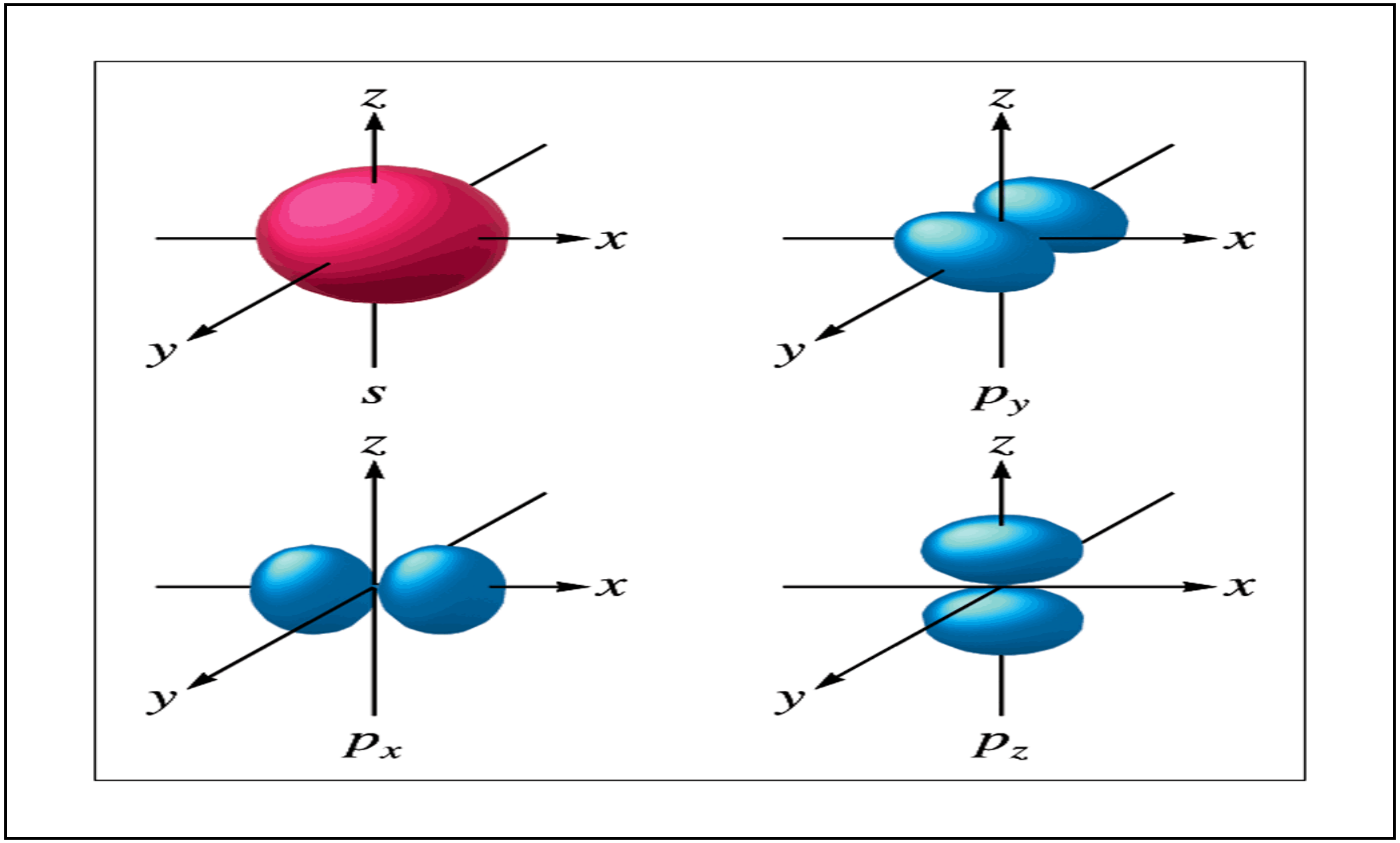
Hybridization

Hybridization is a model which is used to explain the behavior of atomic orbitals during the formation of covalent bonds. When an atom forms a covalent bond with another atom, the orbitals of the atom become rearranged.This rearrangement results in the "mixing" of orbitals.

Hybridisation (or hybridization) is the concept of mixing nonequivalent atomic orbitals into new *hybrid orbitals* (with different energies, shapes, etc., than the component atomic orbitals) . Hybrid orbitals are very useful in the explanation of molecular geometry and atomic bonding properties. Hybrid orbitals have different shapes from original.

When atoms join together to form molecules, their atomic orbitals interact with each other to form hybrid orbitals .

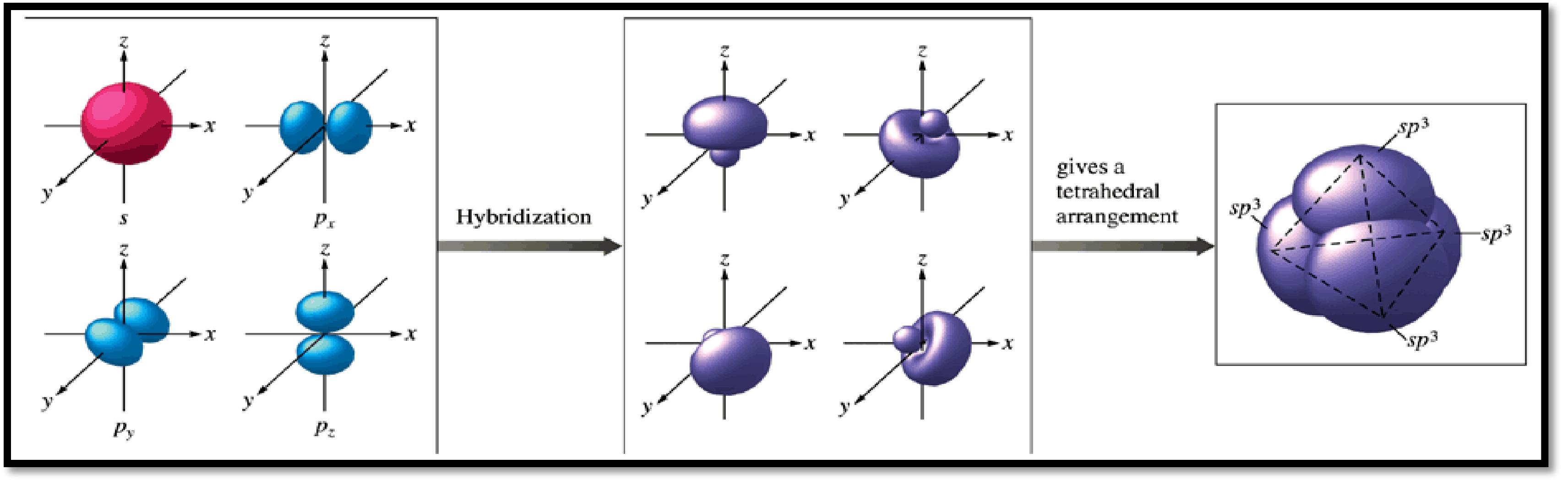
Original atomic orbital



sp^3 hybridisation

E.g. methane, ammonia, water

When C bonds to four other atoms, it hybridized 2s and 2p atomic orbitals to form 4 new sp^3 hybrid orbitalsThe sp^3 orbital shape is between 2s/2p; one large lobe dominates Methane contains 4 equal C - H bonds, therefore the outer shell electrons ($2s^2$ $2p^2$) have merged to form 4 hybrid sp^3 orbitals of equal energy

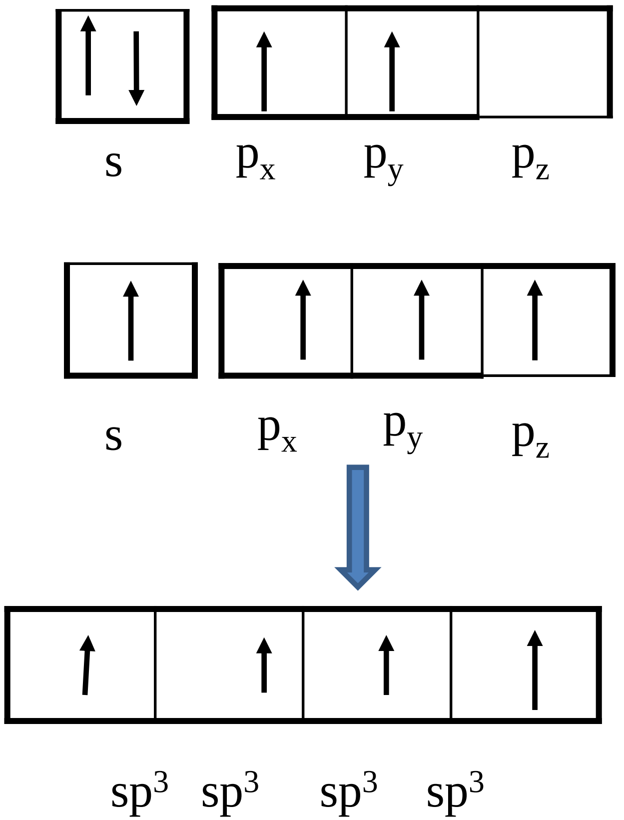


Hybridization

Ground state of C $1s^2\ 2s^2\ sp^2$

Excited state $2s^1 2p^3$

Hybridize oribtales $sp^3\ sp^3\ sp^3\ sp^3$



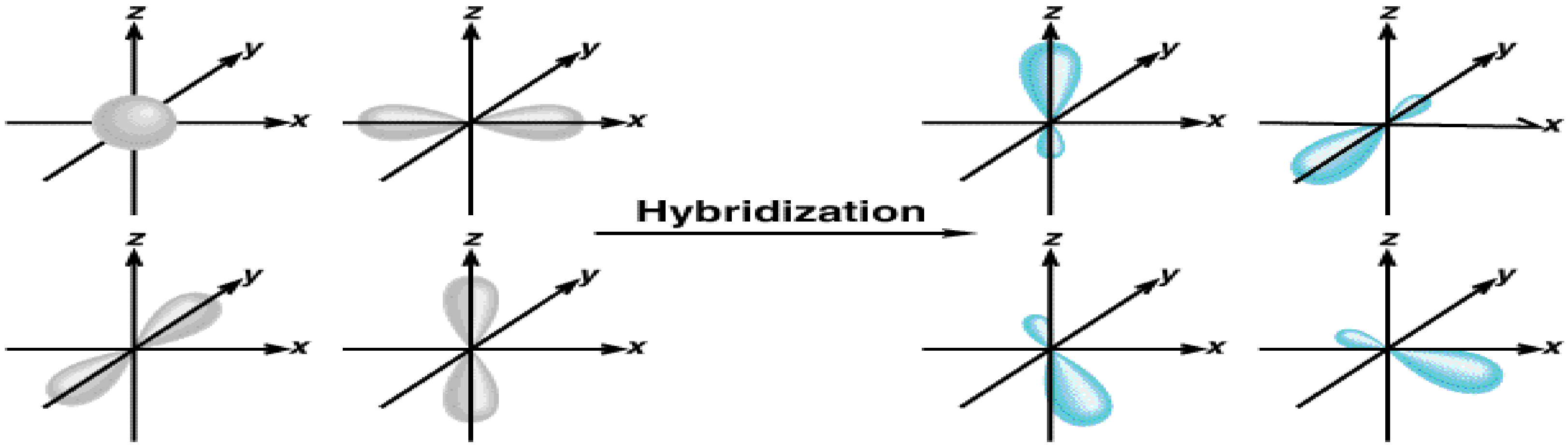
Four sp^3 orbitals of equal length, energy and in tetrahedral shape

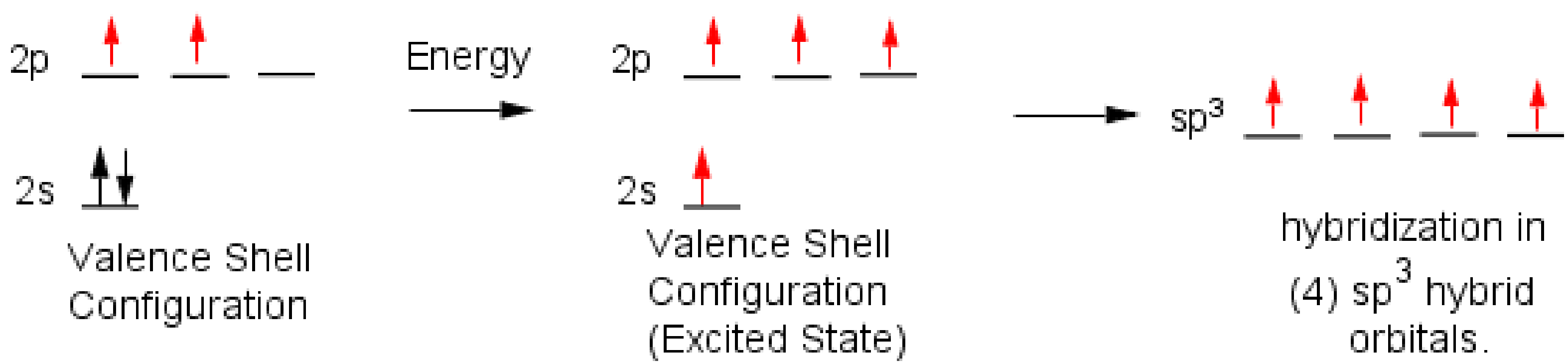
Covalent bonds are formed by:

Overlap of hybrid orbitals with atomic orbitals

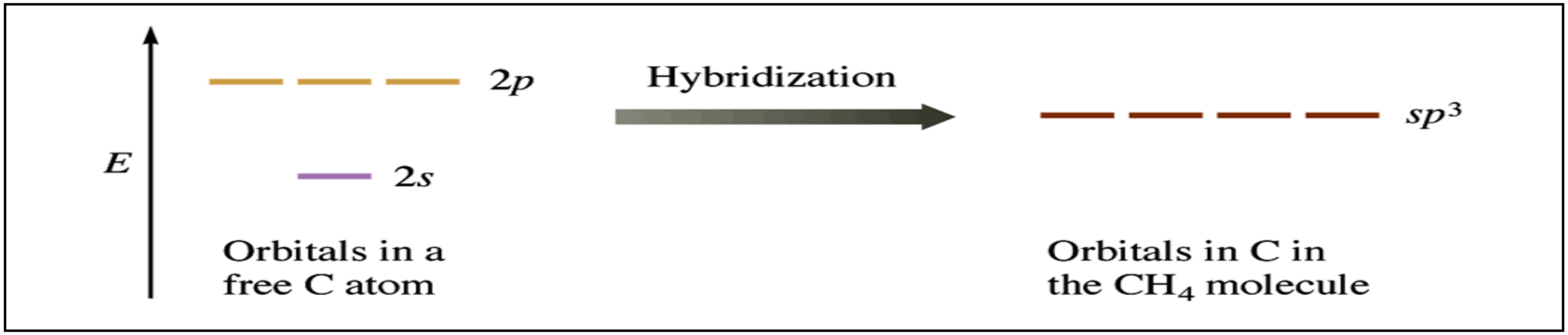
Overlap of hybrid orbitals with other hybrid orbitals

Formation of sp^3 Hybrid Orbitals

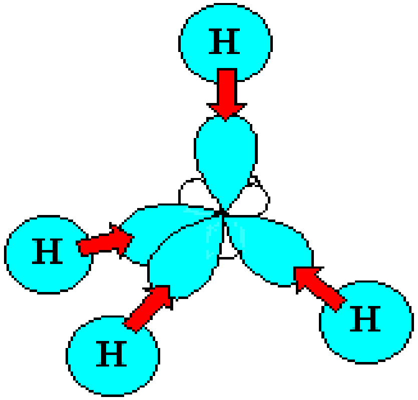


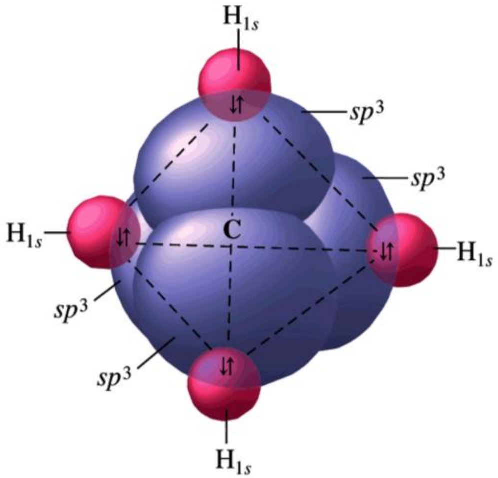


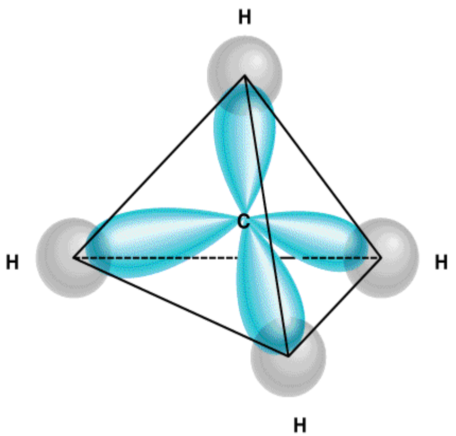
An energy-level diagram showing the formation of four sp^3 orbitals.



The H atoms of methane can only use their 1s orbitals for bonding. The shared electron pair can be found in the overlap area of H1s—Csp^3



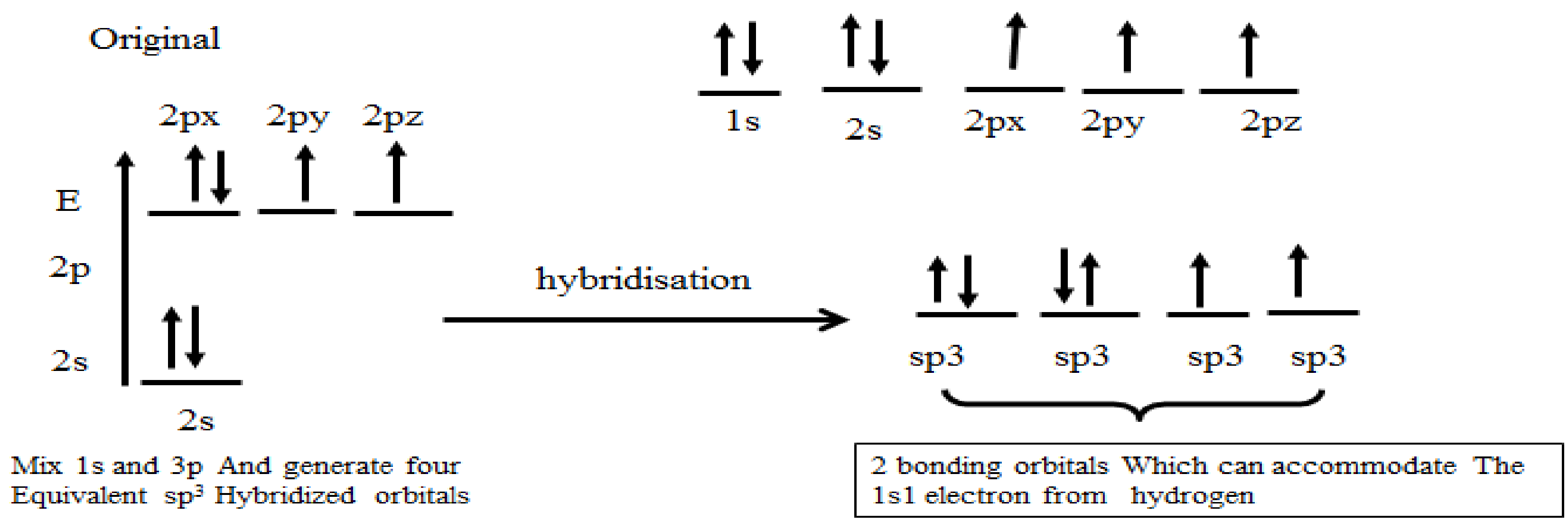


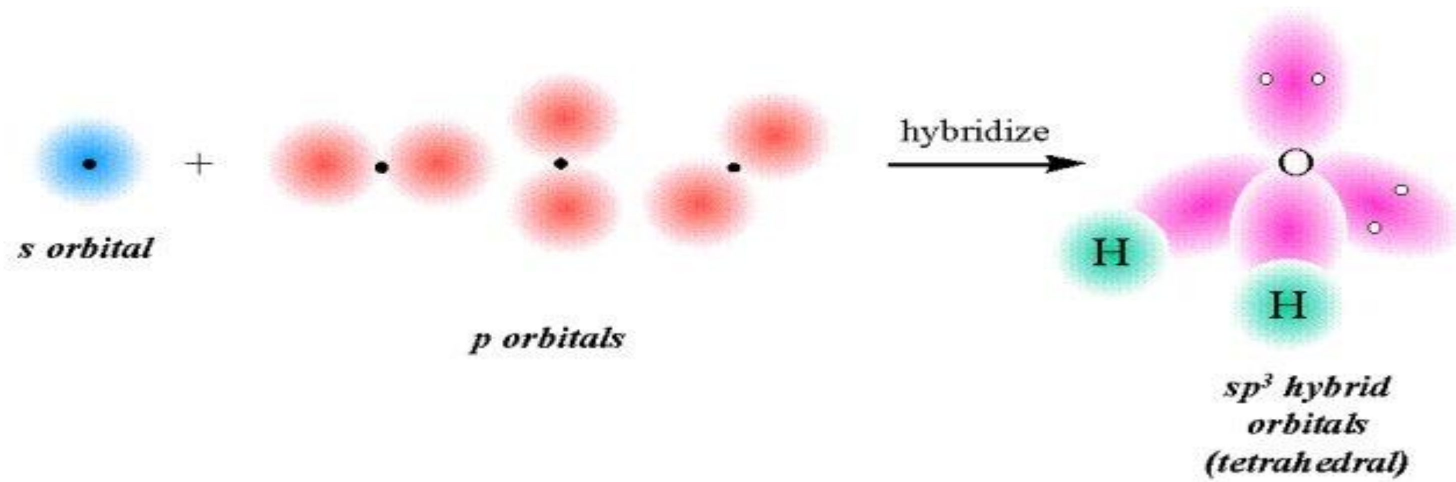


sp^3 hybridisation in water

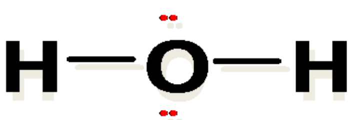
A similar thing occurs in water - 4 sp^3 hybridised orbitals are formed around the oxygen and spread out in a tetrahedral shape . Two of these orbitals contain lone/non-bonded pairs of electrons, and the other two form sigma bonds with the hydrogen atoms. As the non-bonded pairs are closer to the centre of the molecule, they force the two O-H bonds slightly closer together forming a bond angle of 105 º

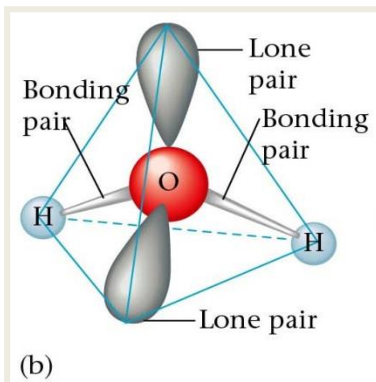
Original orbital $1s^2$ $2s^2$ $2p^4$





Water, H_2O



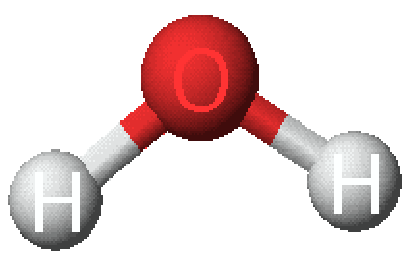


2 bond pairs

2 lone pairs

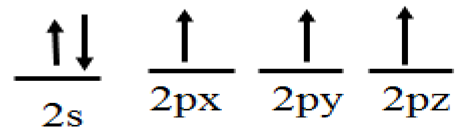
The electron pair geometry is **TETRAHEDRAL**

The molecular geometry is **BENT**.

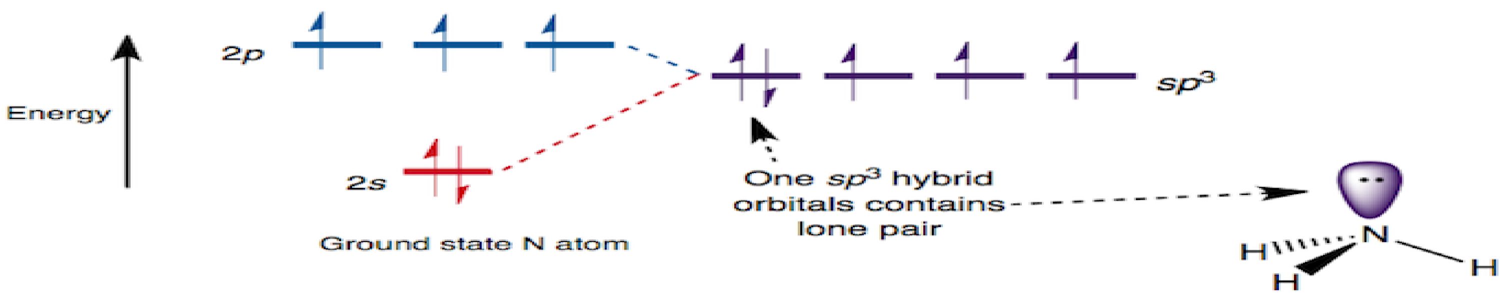


Hybrization in NH3

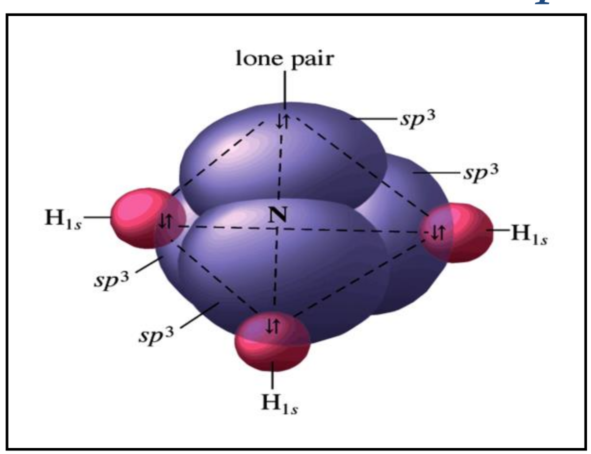
Original orbital $1s^2$ $2s^2$ $2p^3$

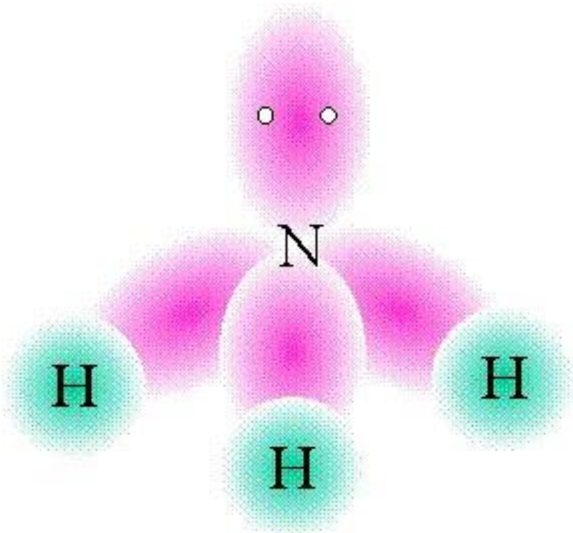


Mix 1s and 3p And generate four Equivalent sp^3 Hybridized orbitals



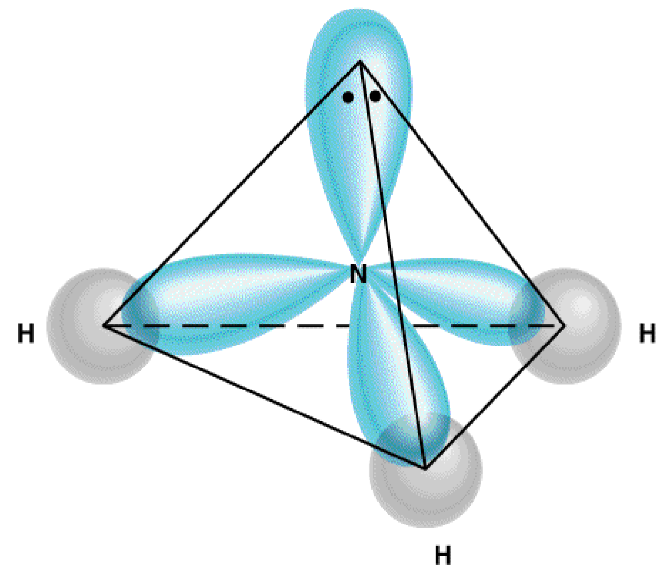
The nitrogen atom in ammonia is *sp*^{3} hybridized.

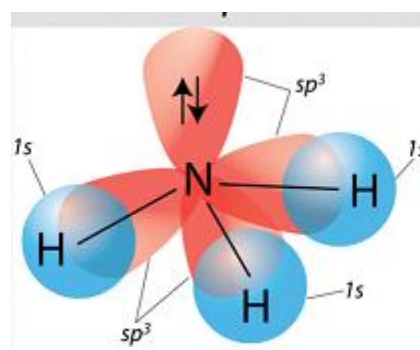




sp^3 hybrid orbitals (tetrahedral)

sp^3 – Hybridized N Atom in NH_3

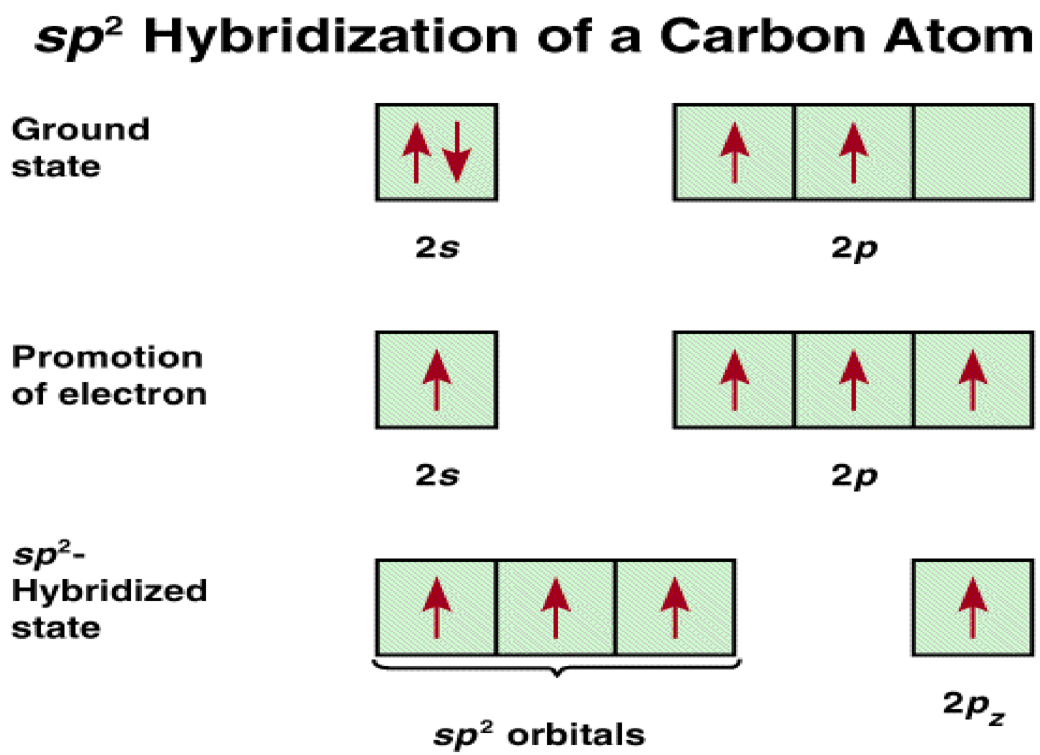




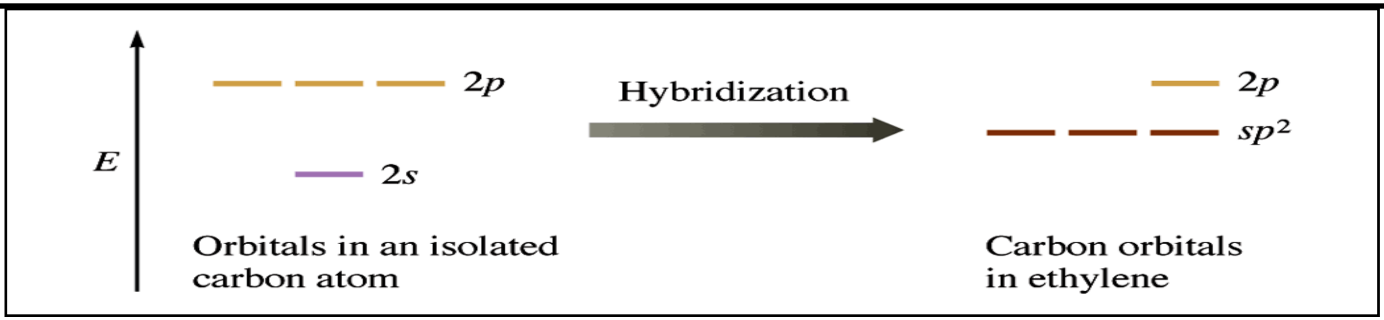
sp^2 hybridisation

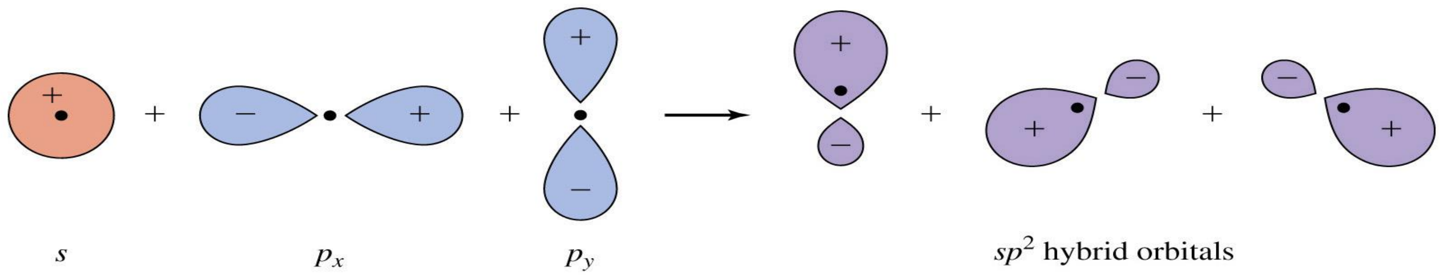
Carbon - sp^2 hybridization

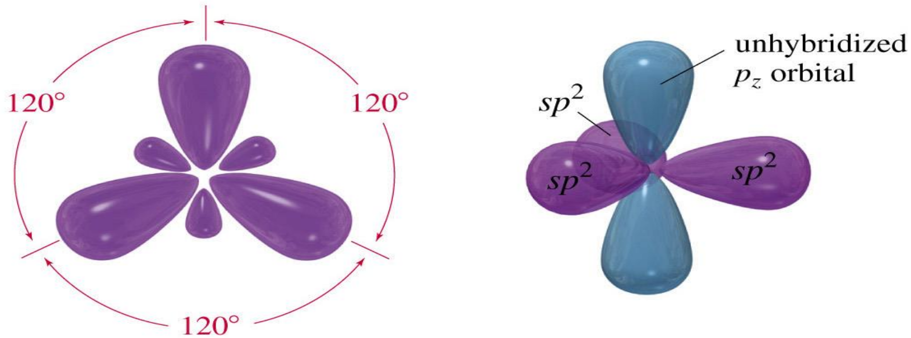
A carbon atom bound to three atoms (two single bonds, one double bond) is sp^2 hybridized and forms a flat *trigonal* or triangular arrangement with 120° angles between bonds.



An orbital energy-level diagram for sp^2 hybridization. Note that one p orbital remains unchanged.



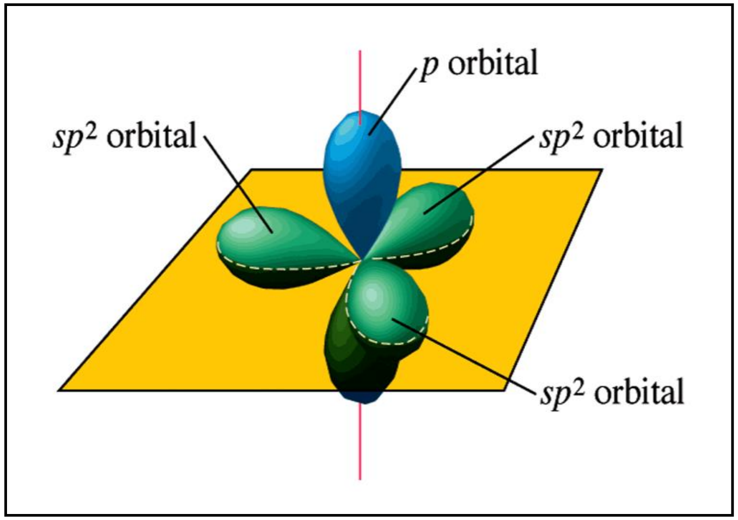


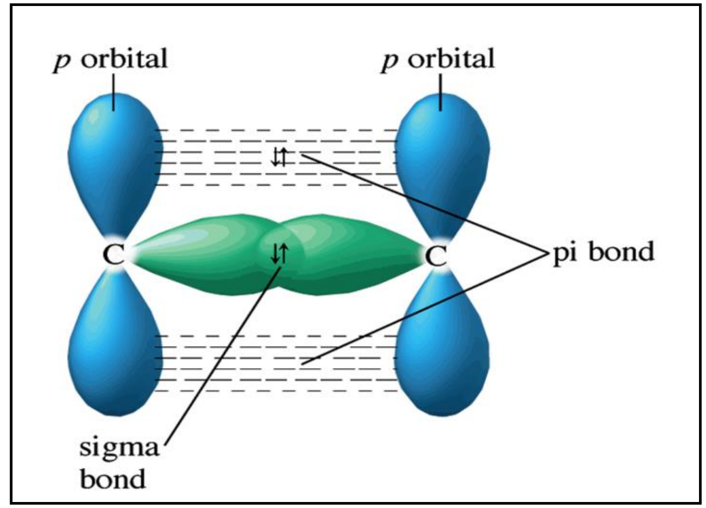


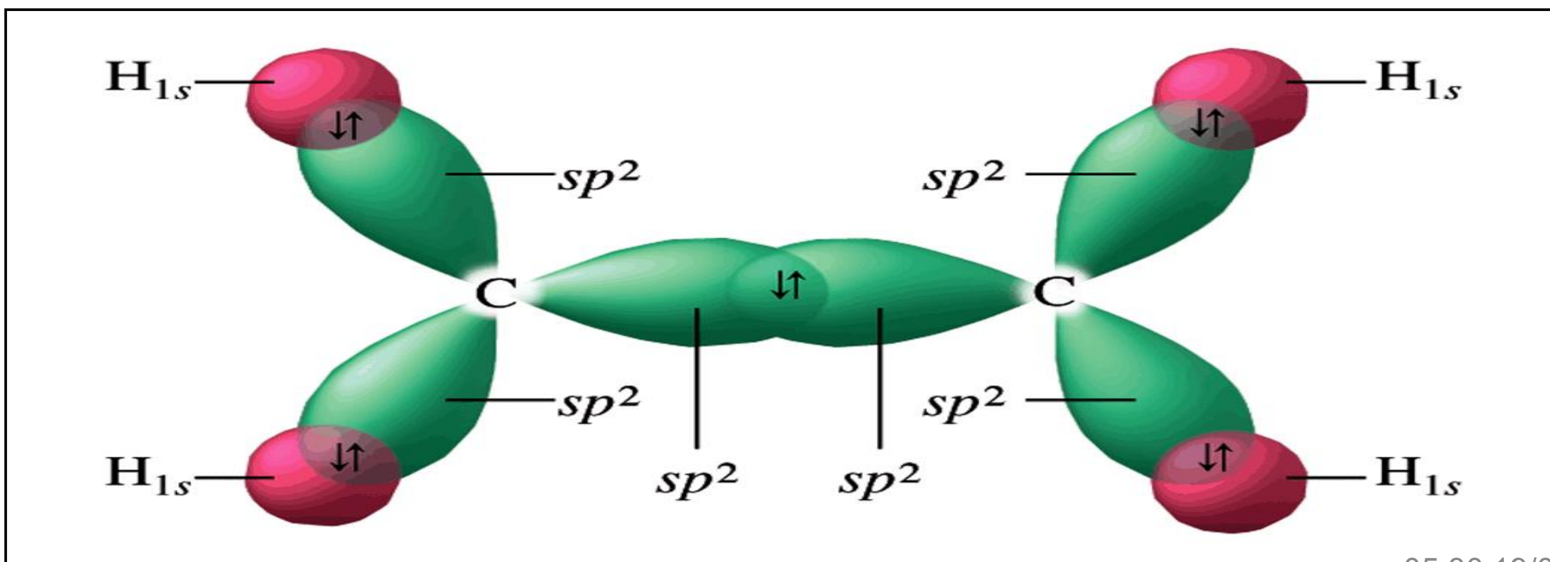
three sp^2 hybrid orbitals superimposed

sp^2 hybrid carbon atom (viewed from the side)

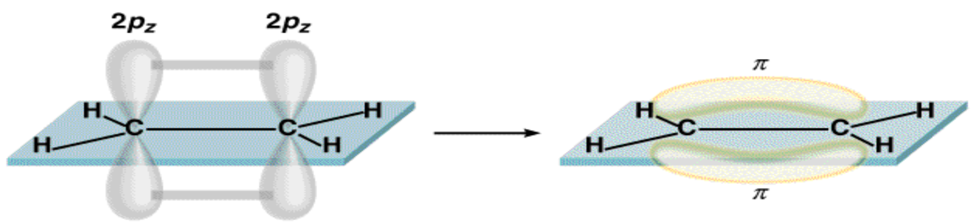
When an *s* and two *p* orbitals are mixed to form a set of three sp^2 orbitals, one *p* orbital remains unchanged and is perpendicular to the plane of the hybrid orbitals.

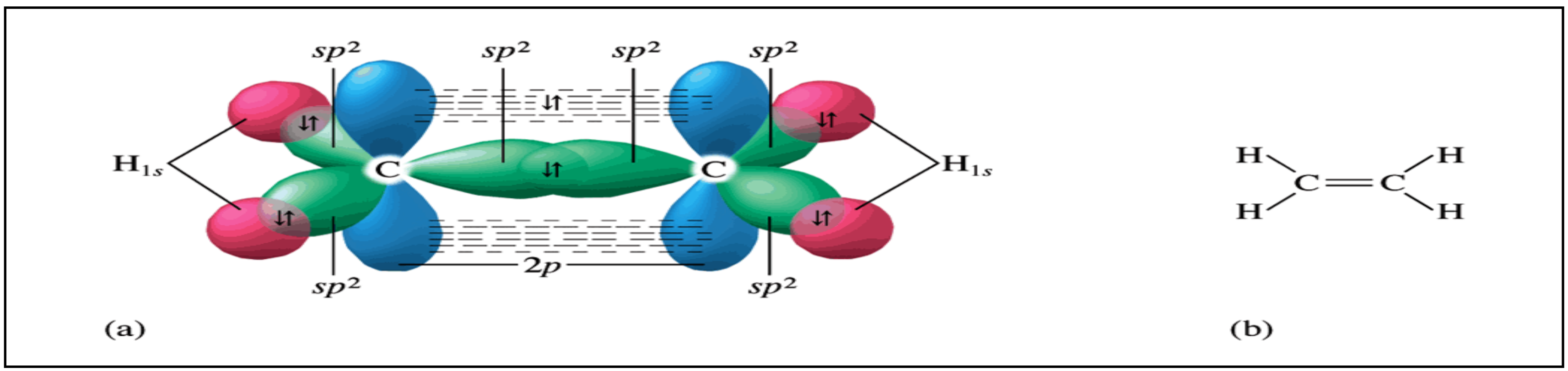




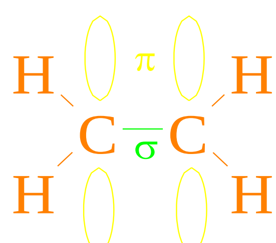


Pi Bond Formation in the Ethylene Molecule





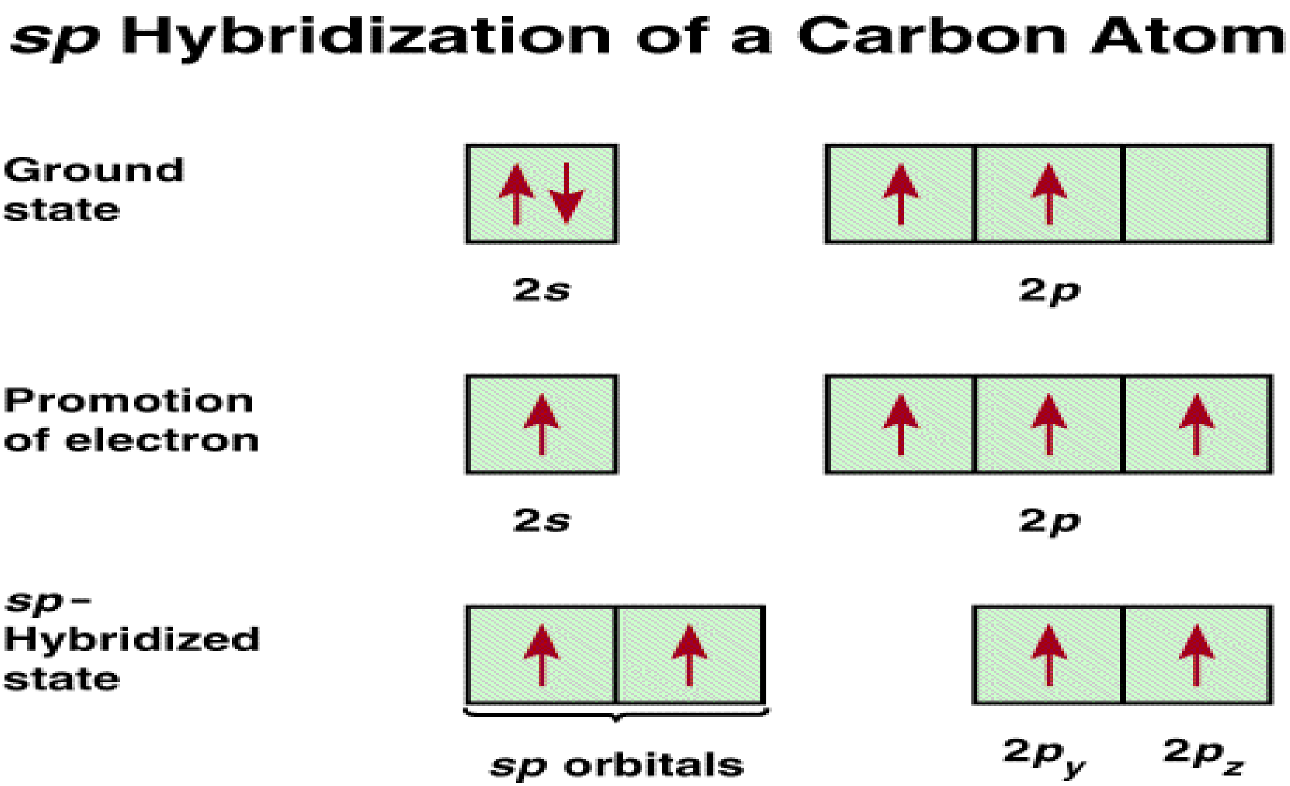
sigma (σ) bond centers along the internuclear axis. pi (π) bond occupies the space above and below the internuclear axis.



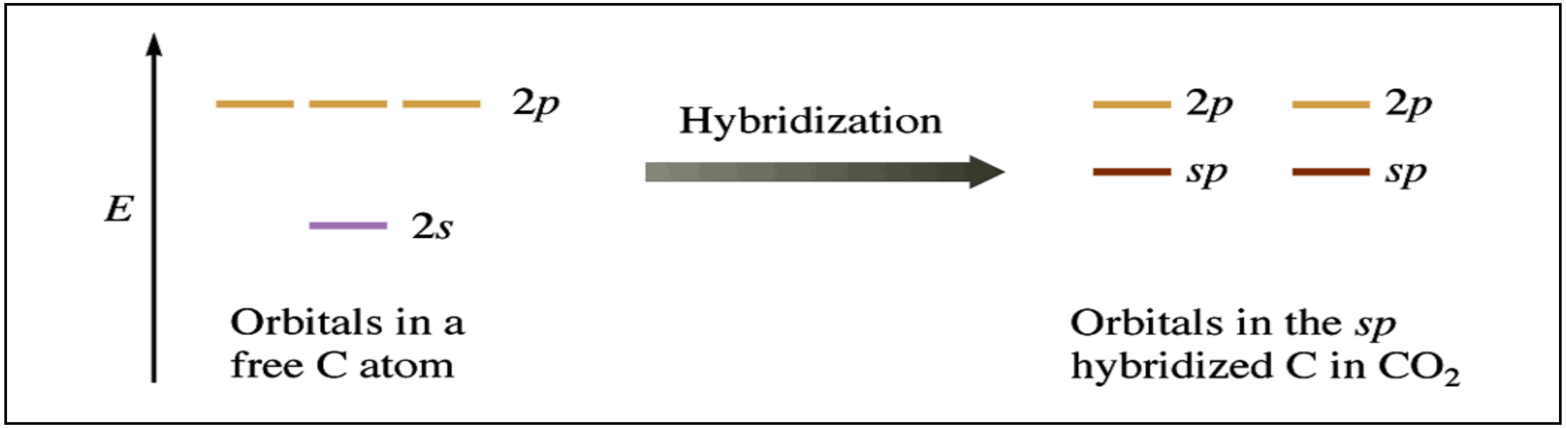
sp hybridization

Carbon - sp hybridization

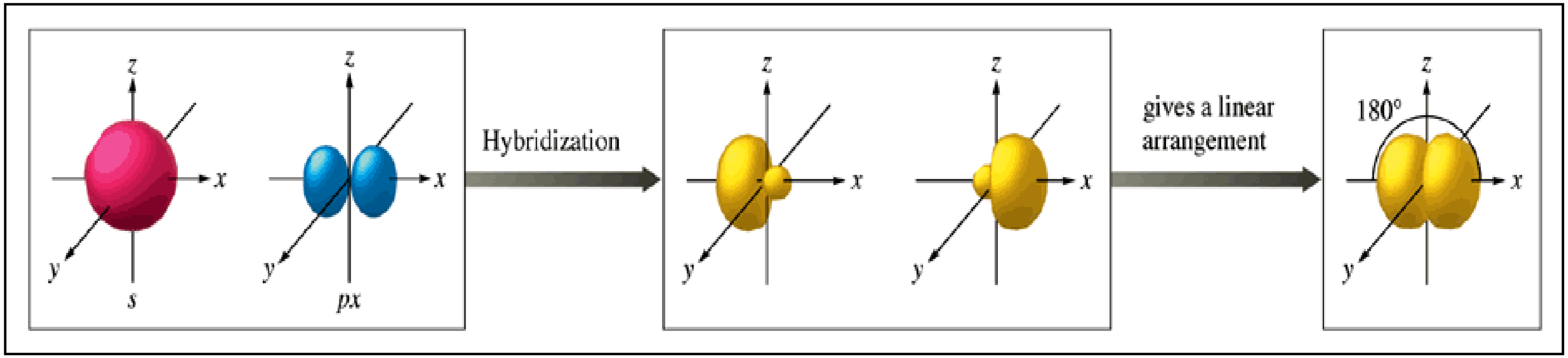
A carbon atom bound to two atoms (one single bonds, two double bond) is sp hybridized and forms a linear with 180° angles between bonds



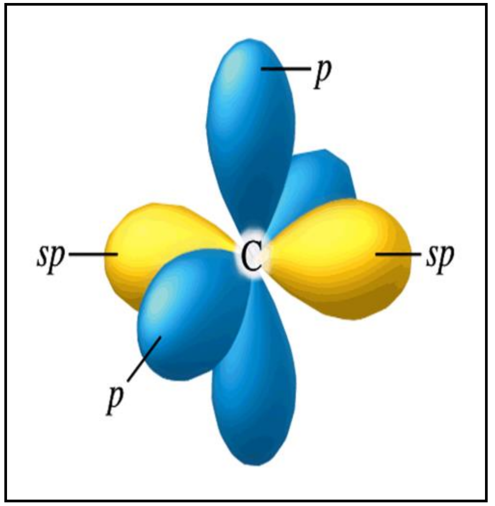
The orbital energy-level diagram for the formation of *sp* hybrid orbitals on carbon.



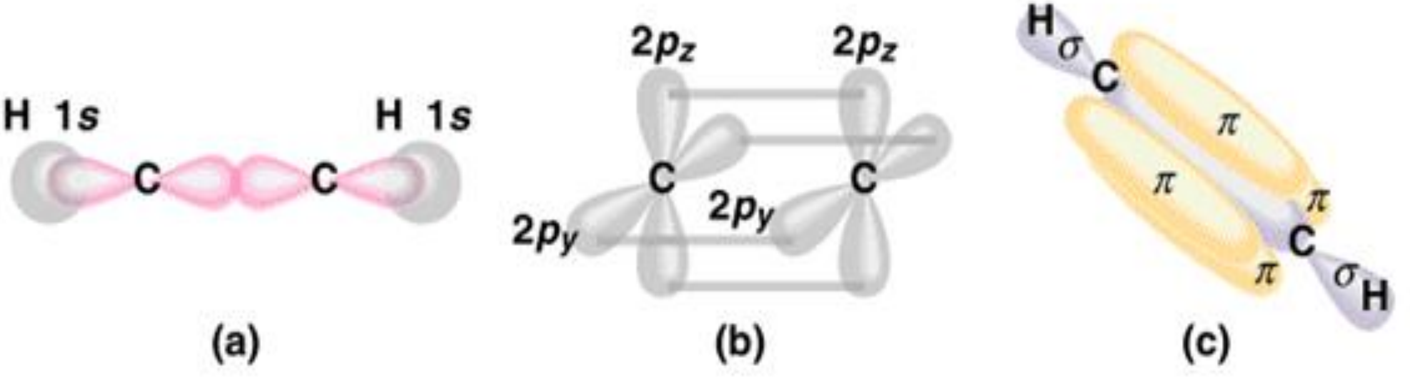
When one *s* orbital and one *p* orbital are hybridized, a set of two *sp* orbitals oriented at 180 degrees results.



The orbitals of an *sp* hybridized carbon atom.

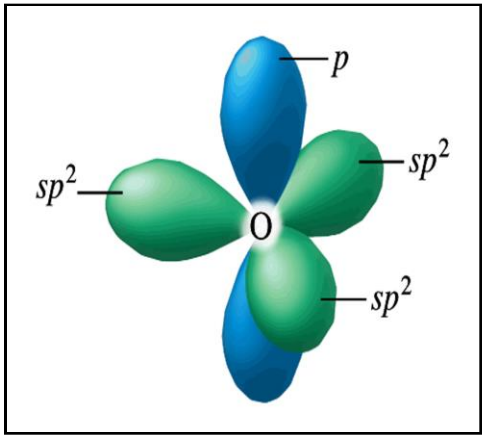


Bonding in Acetylene

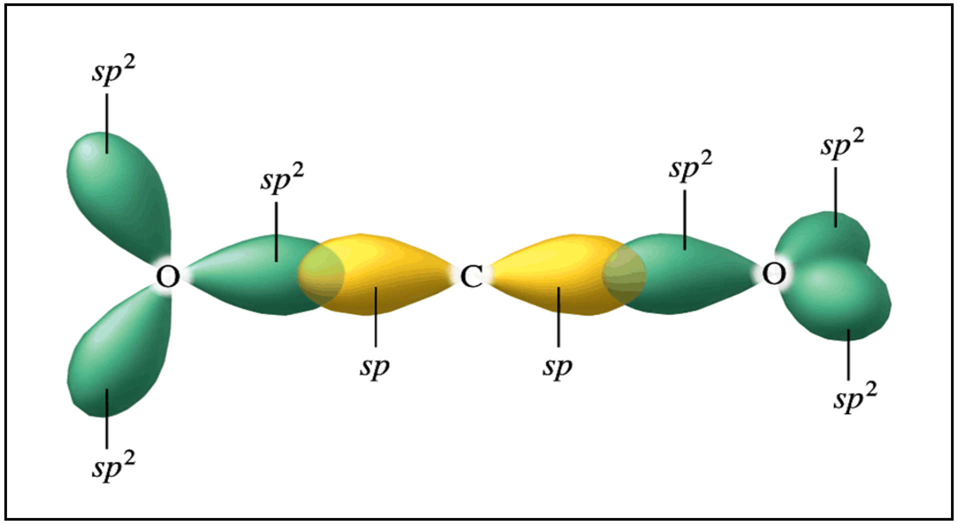


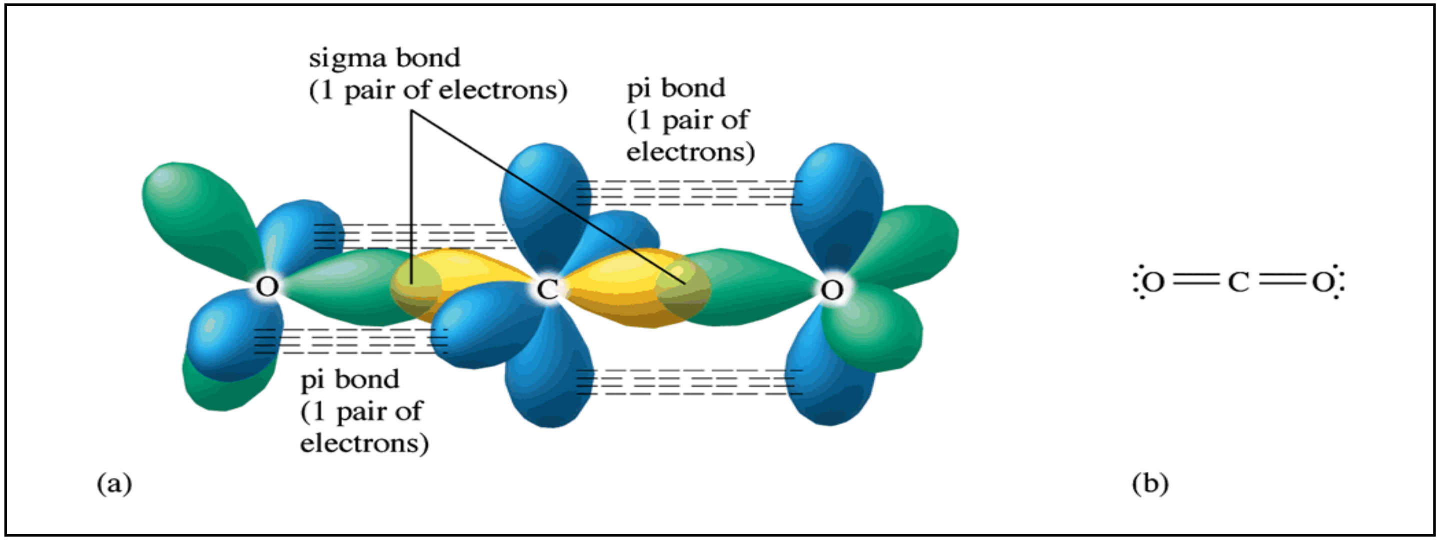
The orbital arrangement for an *sp*^{2} hybridized oxygen atom to form CO_2.

$^8O\ 1s^2 2s^2 2p^4$



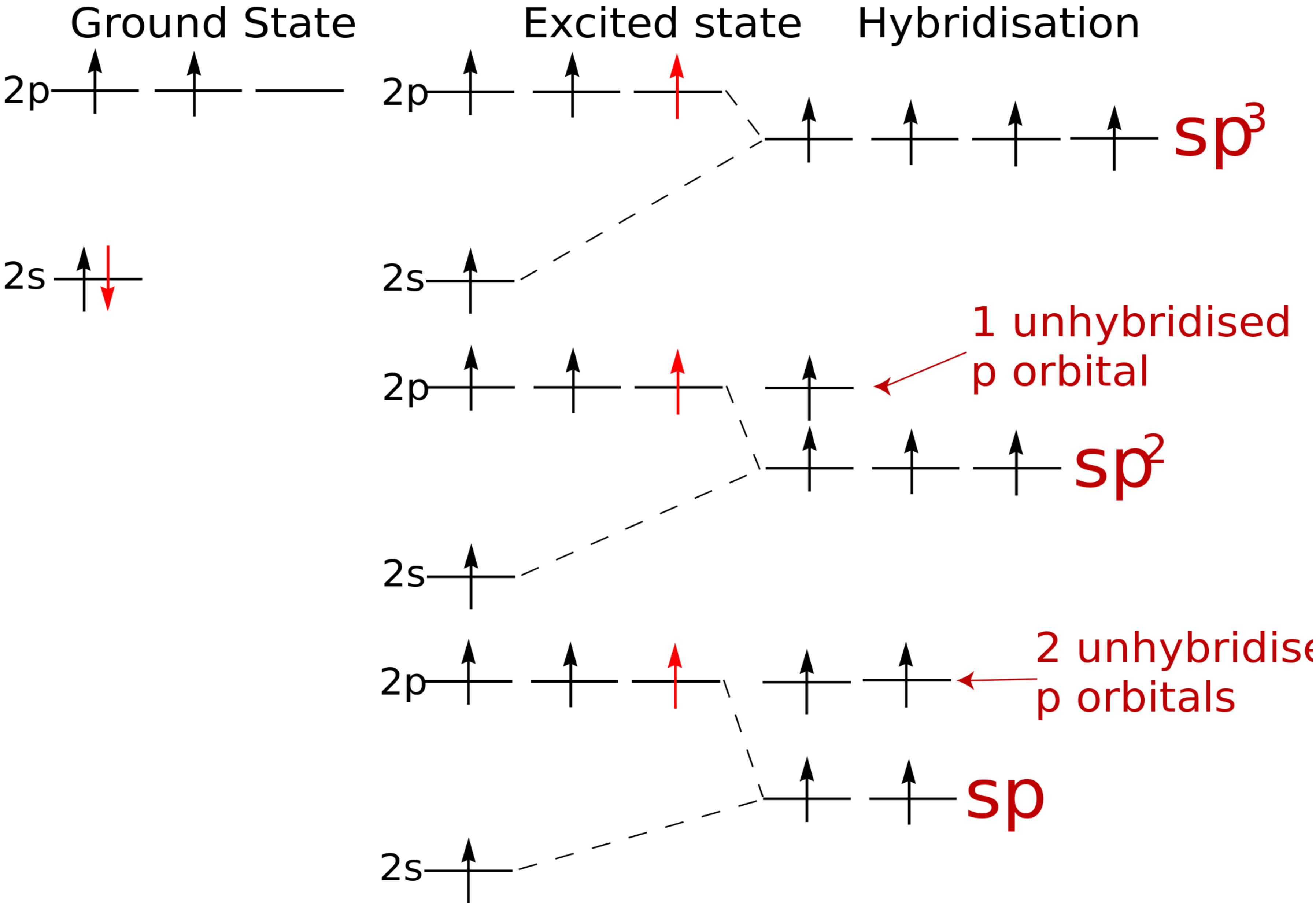
The hybrid orbitals in the CO_2 molecule.



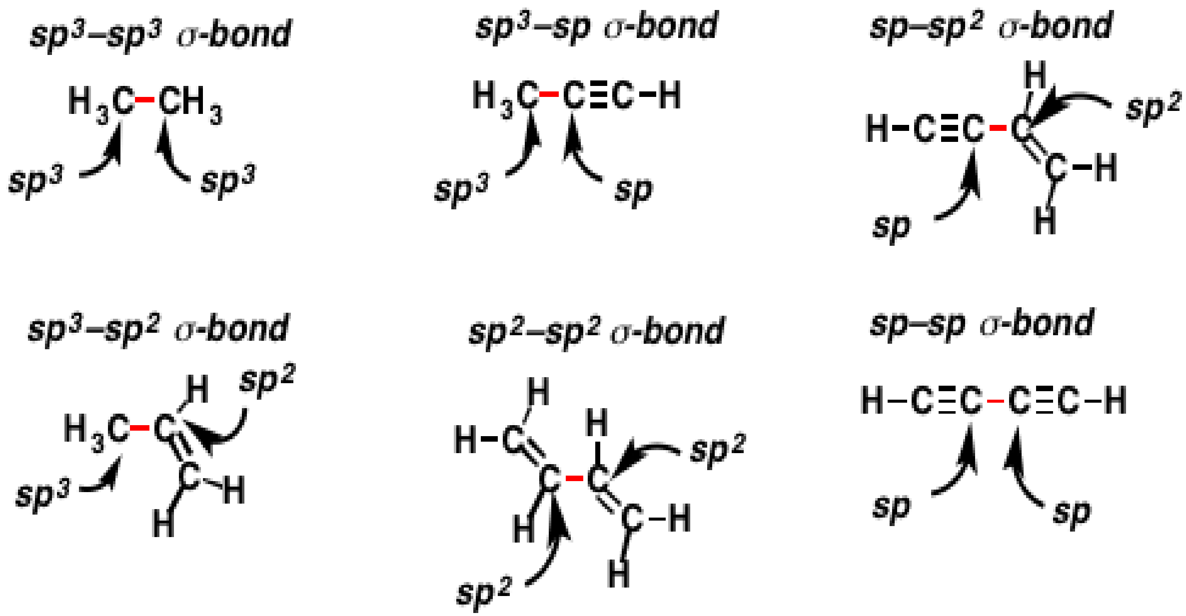


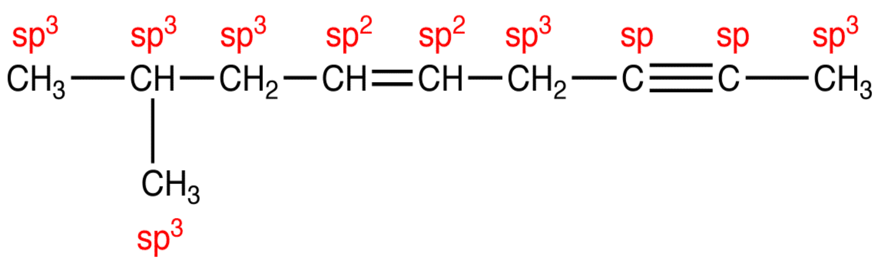
Sigma (σ) and Pi Bonds (π)

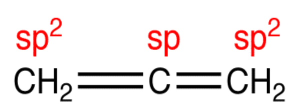
Single bond	1 sigma bond
Double bond	1 sigma bond and 1 pi bond
Triple bond	1 sigma bond and 2 pi bonds


Ground State
Excited state
Hybridisation
2p
2s
2p
2s
sp3
2p
2s
1 unhybridised
p orbital
sp2
2p
2s
2 unhybridise
p orbitals
sp

The six types of carbon-carbon σ-bonds







Electronegativity

Electronegativity:

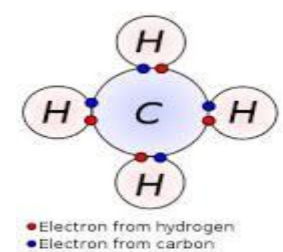
a measure of an atom's attraction for the electrons it shares with another atom in a chemical bond

Pauling scale

generally increases left to right in a row

generally increases bottom to top in a column

A **covalent bond**, also called a molecular **bond**, is a chemical**bond** that involves the sharing of electron pairs between atoms. These electron pairs are known as shared pairs or **bonding**pairs, and the stable balance of attractive and repulsive forces between atoms, when they share electrons, is known as **covalent bonding**.



We divide covalent bonds into.

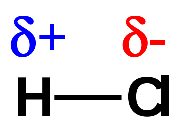
1- nonpolar covalent bonds. electronegativity between atoms are equal .

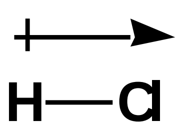
2- polar covalent bonds the difference in electronegativity between atoms .

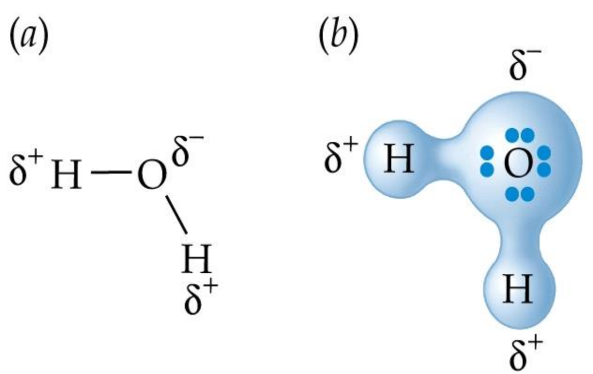
an example of a polar covalent bond is that of H-Cl

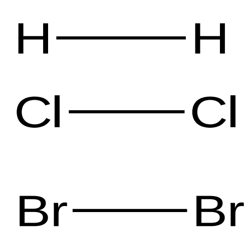
the difference in electronegativity between Cl and H is 3.0 - 2.1 = 0.9

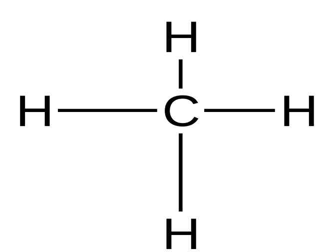
we show polarity by using the symbols d+ and d-, or by using an arrow with the arrowhead pointing toward the negative end and a plus sign on the tail of the arrow at the positive end .





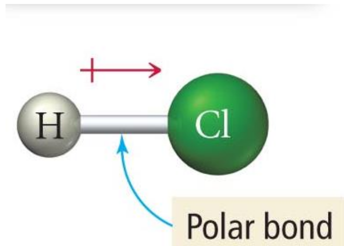


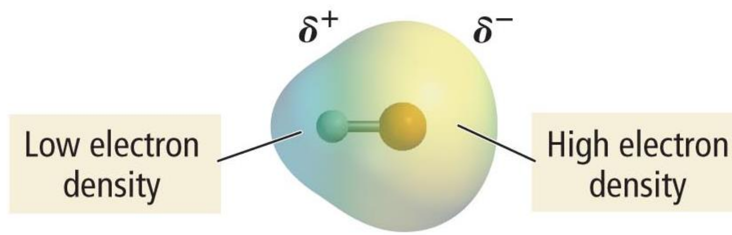


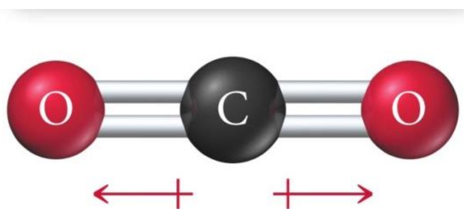


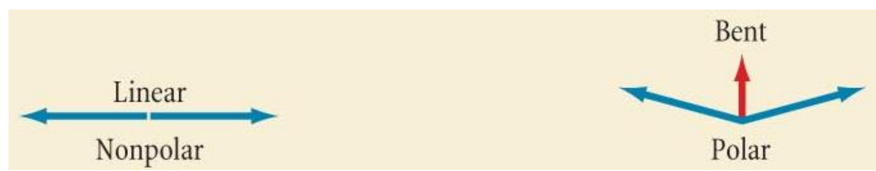
III.Polar Bonds

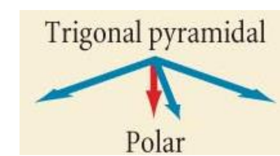
A. Any bond between atoms of different electronegativities is polar
Electrons concentrate on one side of the bond
One end of the molecule is (+) and one end is (-)

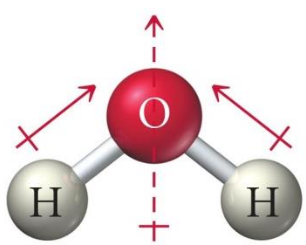


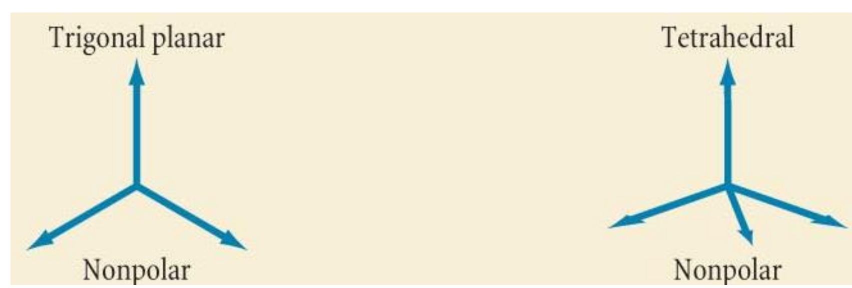












Polar molecules

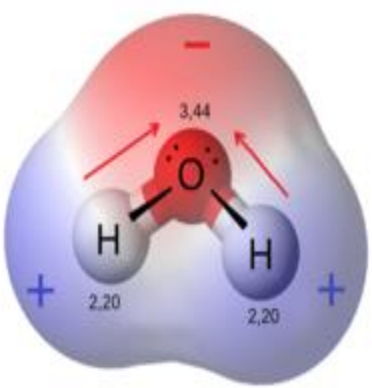
polarity is a separation of electric charge leading to a molecule or its chemical groups having an electric dipole or multipole moment.

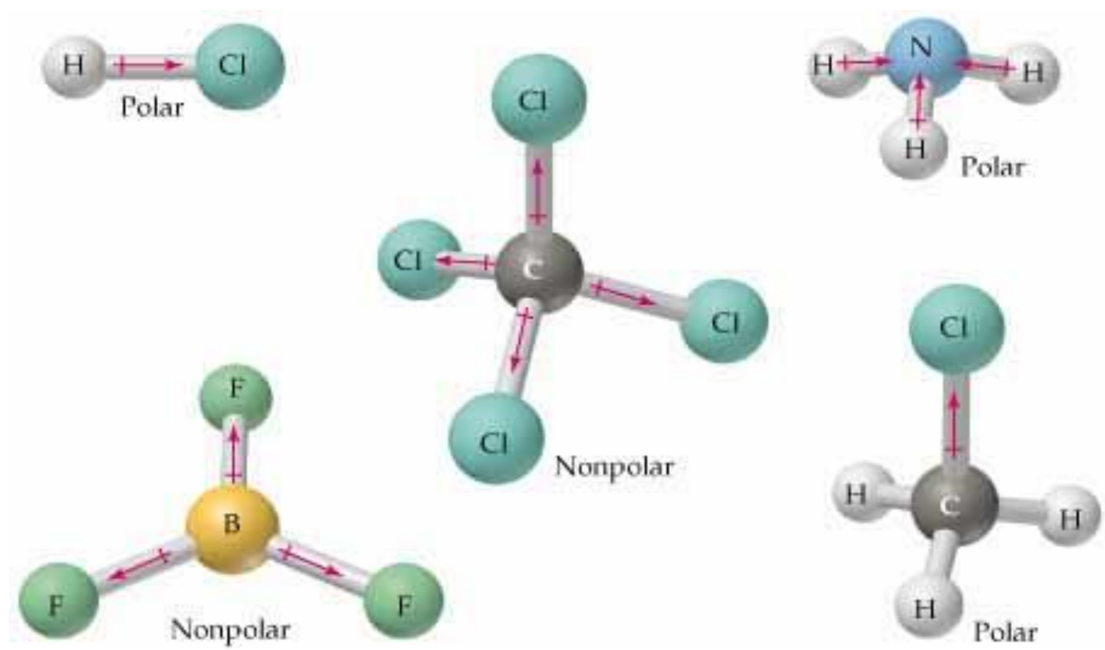
Polar molecules must contain polar bonds due to a difference in electronegativity between the bonded atoms. A polar molecule with two or more polar bonds must have an asymmetric geometry so that the bond dipoles do not cancel each other.

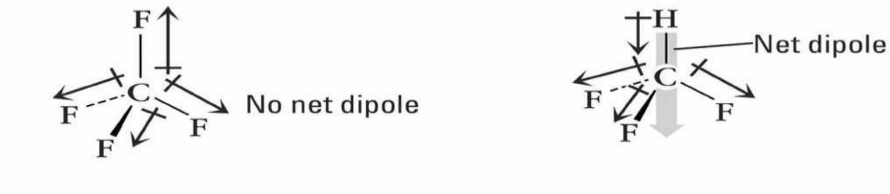
Polar molecules interact through dipole–dipole intermolecular forces and hydrogen bonds. Polarity underlies a number of physical properties including surface tension, solubility, and melting and boiling points.

Polar molecules

If the bond dipole moments of the molecule do not cancel, the molecule is polar. For example, the water molecule (H_2O) contains two polar O−H bonds in a bent (nonlinear) geometry. The bond dipole moments do not cancel, so that the molecule forms a molecular dipole with its negative pole at the oxygen and its positive pole midway between the two hydrogen atoms. In the figure each bond joins the central O atom with a negative charge (red) to an H atom with a positive charge (blue).

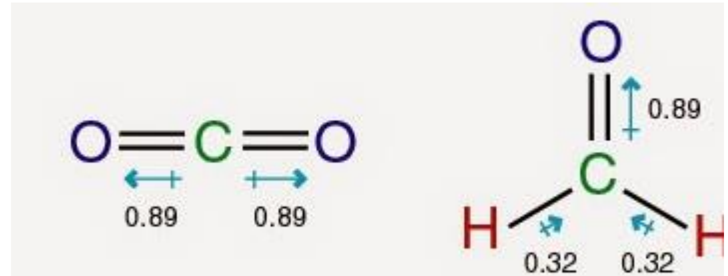


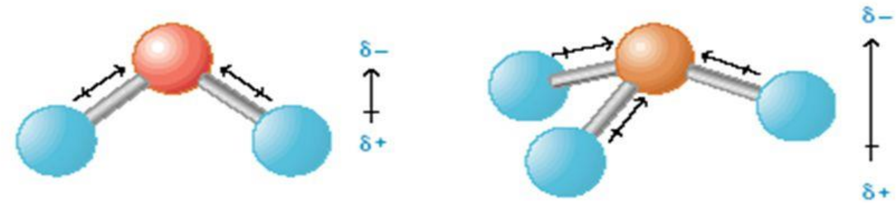




CF_4 is nonpolar

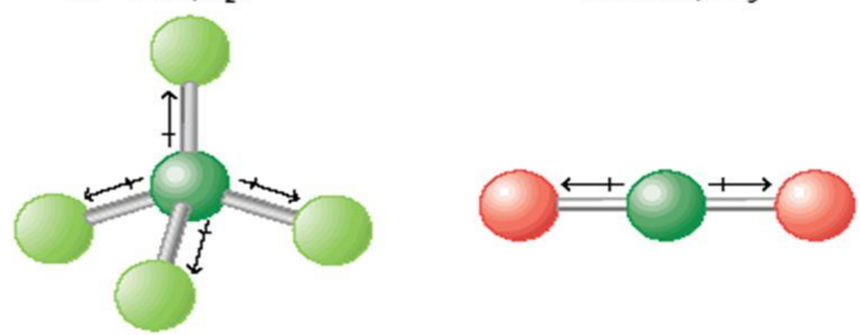
CHF_3 is polar





(a) Water, H_2O

Ammonia, NH_3



(b) Carbon tetrachloride, CCl_4
(no molecular dipole)

Carbon dioxide, CO_2
(no molecular dipole)