Chapter II

Hybridization in hydrocarbons

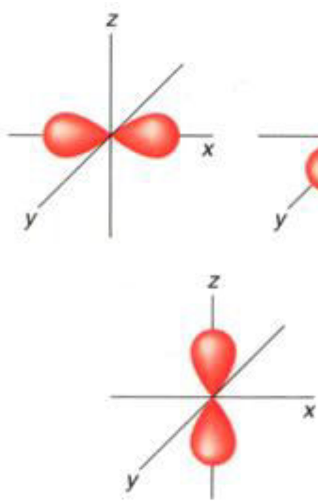
Remember!!!

Orbital ("electron cloud"): Region in space where there is 90% probability of finding an electron

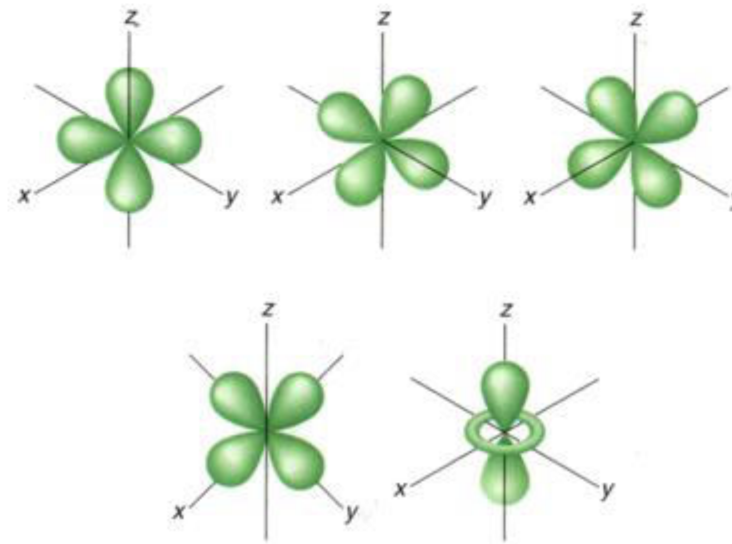
Electron Configuration:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^6 \ldots$

s orbital



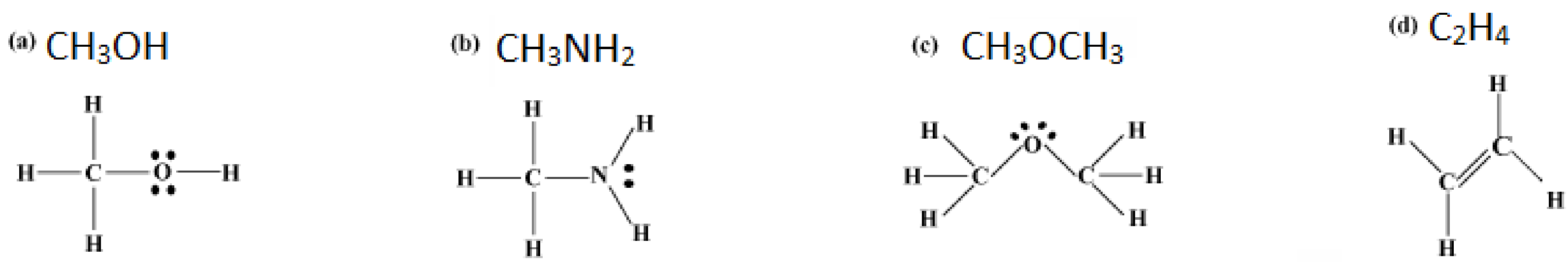
p orbitals



d orbitals

Atomic Orbitals

- Molecules = atoms bound together by sharing e- pairs between atomic orbitals
- **Lewis structures:** are diagrams that show the bonding between atoms of a molecule and the lone pairs of electrons that may exist in the molecule.



- Linear combination of atomic orbitals:

 - between different atoms is bond formation

- on the same atom is hybridization

- **Hybridization** combination of different atomic orbitals on the same atom to form new molecular orbitals (MO) having the same energy.
- Number of combined atomic orbitals = number of resulted hybrid orbitals.

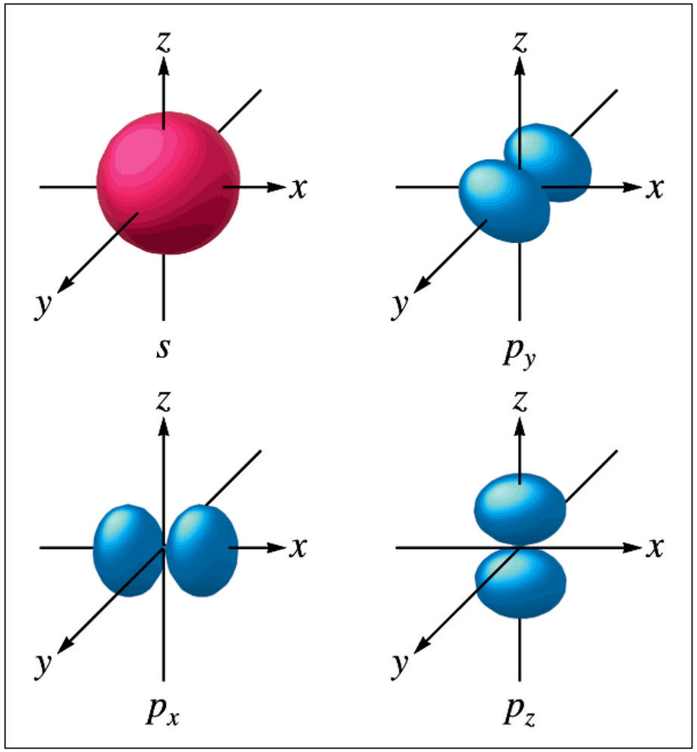
1- sp^3 Hybridization: combination of an s orbital with 3 p orbitals to form four sp^3 hybrid orbitals

Methane, CH_4, will be our example

Electron configuration of H, C:

$_1H = 1s^1$ $_6C = 1s^2, 2s^2, 2p^2$

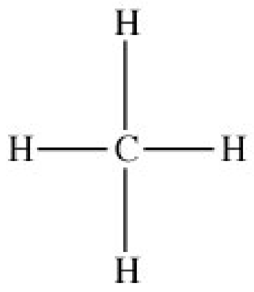
Bonding only involves valence e- H = 1s C = 2s, 2p



If we use pure atomic orbitals directly, the predicted shape would have:

a. One C2s--H1s bond would be shorter than others

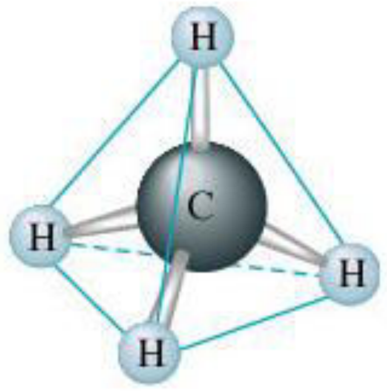
b. Three C2p--H1s bonds would be at right angles to each other



However, CH_4 is tetrahedral, symmetric

Free elements (C) use pure atomic orbitals

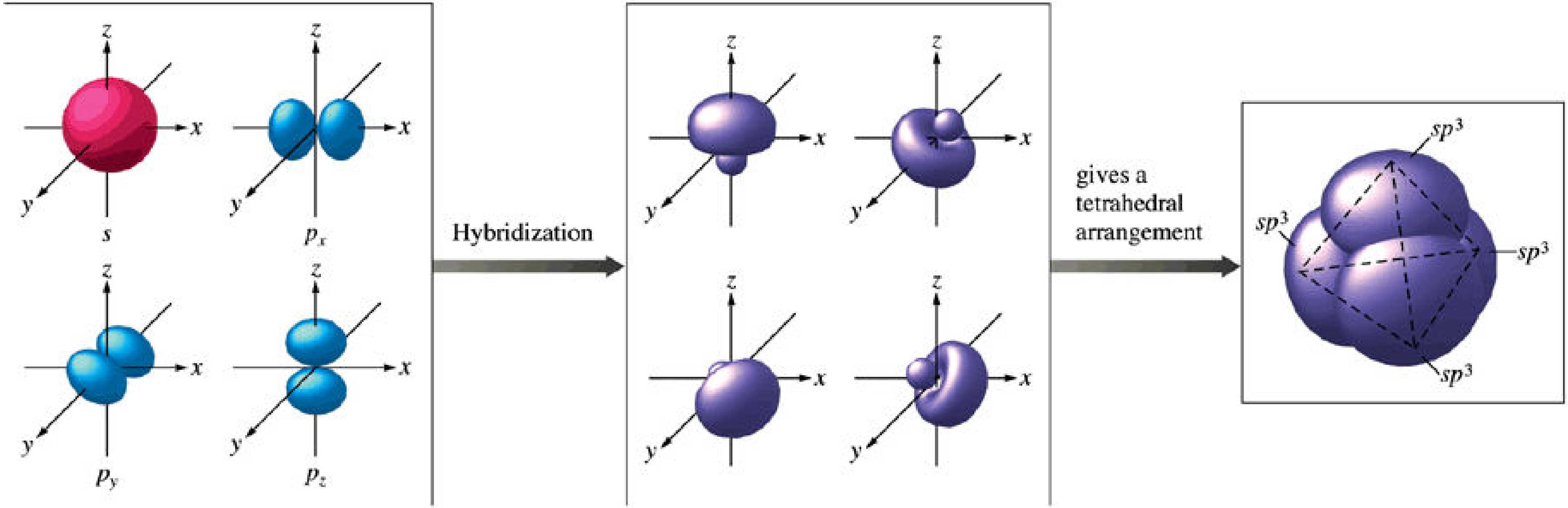
Elements involved in bonding will modify their orbitals to reach the minimum energy configuration



When C bonds to four other atoms, it hybridized its 2s and 2p atomic orbitals to form 4 new sp^3 hybrid orbitals

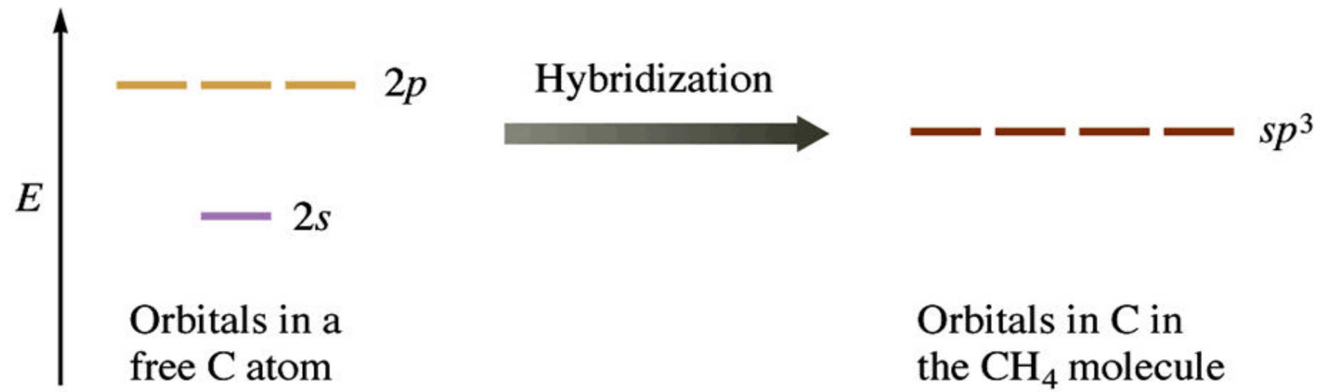
a. The sp^3 orbital shape is between 2s/2p; one large lobe dominates

b. When you hybridize atomic orbitals, you always get an equal number of new molecular orbitals

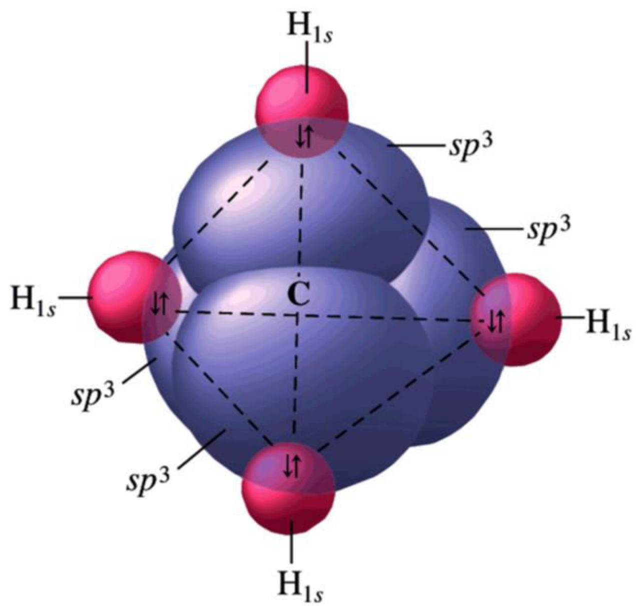


The sp^3 orbitals are lower in energy than the original atomic orbitals (s, p).

The four sp^3 orbitals have the same energy (degenerate).



The H atoms of methane can only use their 1s orbitals for bonding.



Steric number:

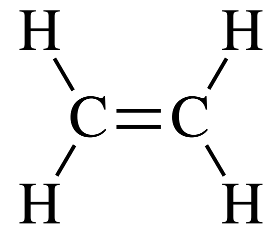
The **steric number** of a molecule is the number of atoms bonded to the central atom of a molecule plus the number of lone pairs on the central atom.

if Steric no comes to be **4**, there is sp^3 hybridization in the atom. if steric no comes to be **3**, there is sp^2 hybridization in the atom. if steric no comes to be **2**, there is sp hybridization in the atom.

Q1. predict the hybridization in N atom and O atom in NH_3 and H_2O

NH_3 and H_2O have sp^3 hybridization.

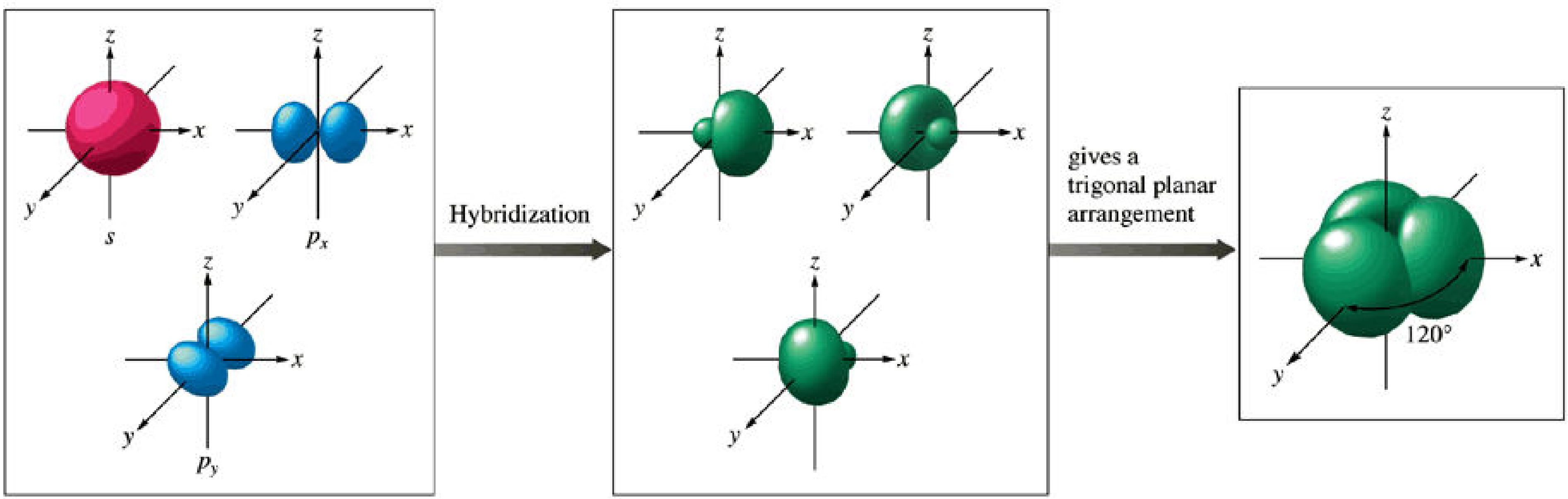
sp^2 Hybridization: combination of an s orbital with 2 p orbitals to form three sp^2 hybrid orbitals



C_2H_4, ethylene is our example

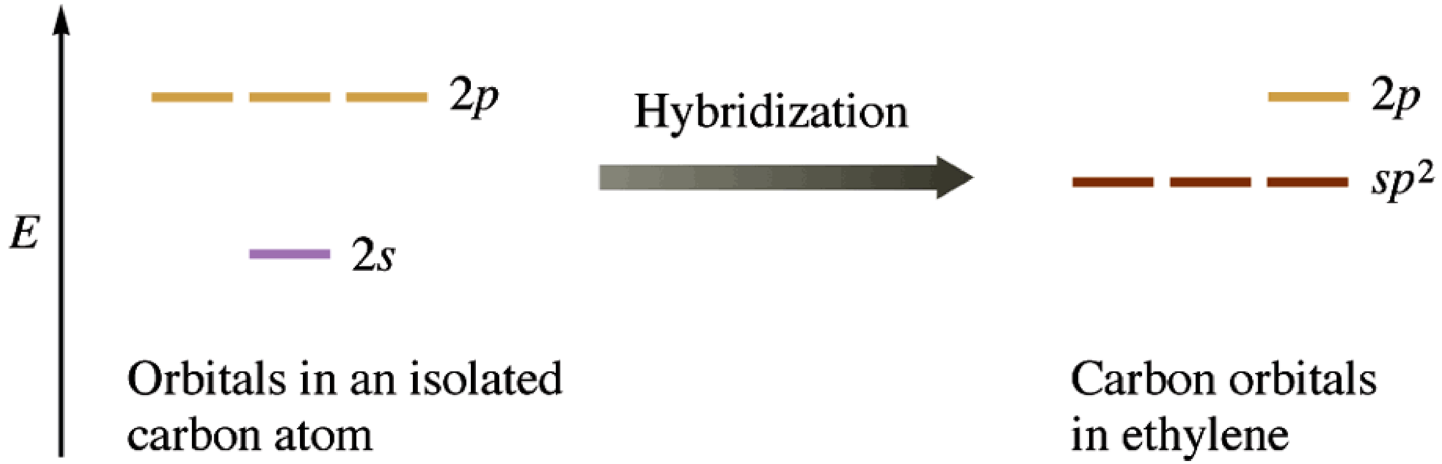
H atoms still can only use 1s orbitals

C atom hybridizes 2s and two 2p orbitals to form 3 sp^2 hybrid orbitals



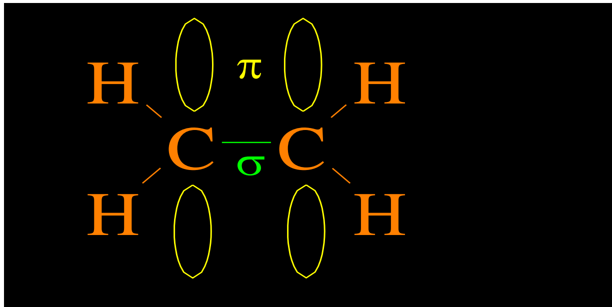
The new sp^2 orbitals are degenerate and in the same plane

One 2p orbital is left unchanged and is perpendicular to that plane

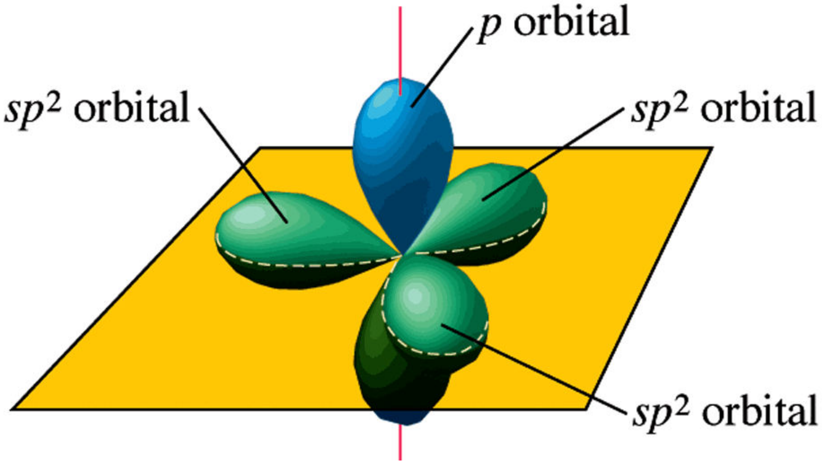


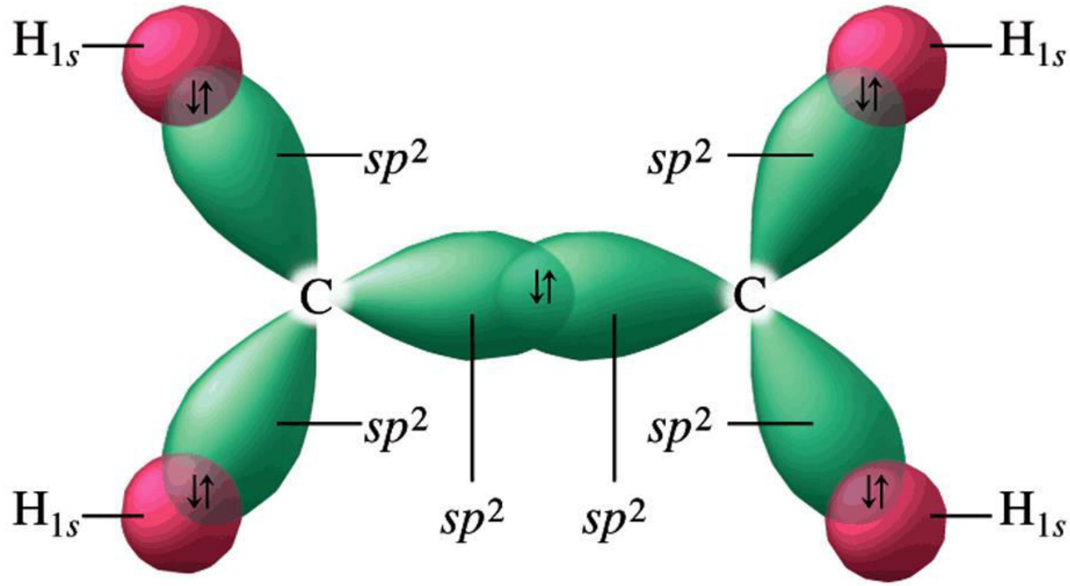
One C—C bond of ethylene forms by overlap of an sp^2 orbital from each of the two sp^2 hybridized C atoms. This is a sigma (σ) bond because the overlap is along the internuclear axis.

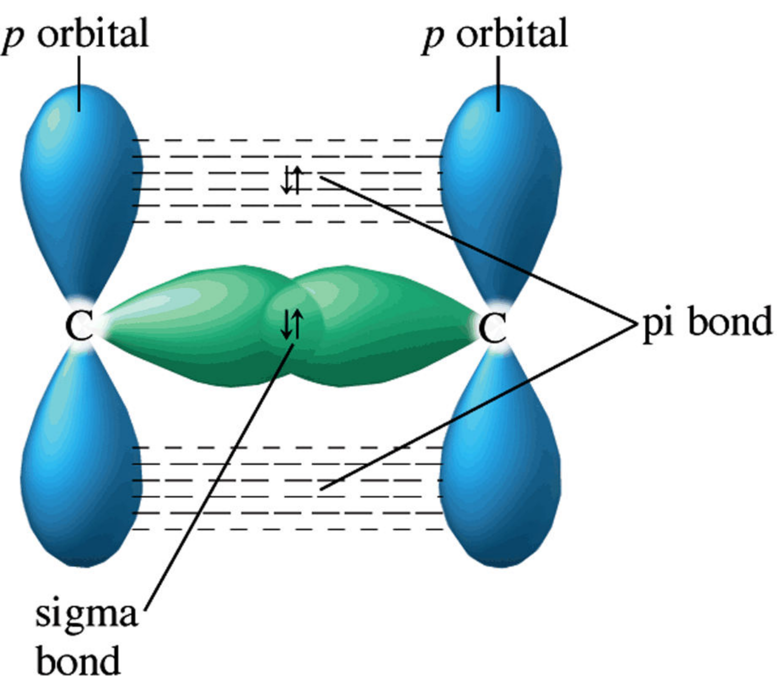
The second C—C bond forms by overlap of the remaining single 2p orbital on each of the carbon atoms. This is a pi (π) bond because the overlap is perpendicular to the internuclear axis.

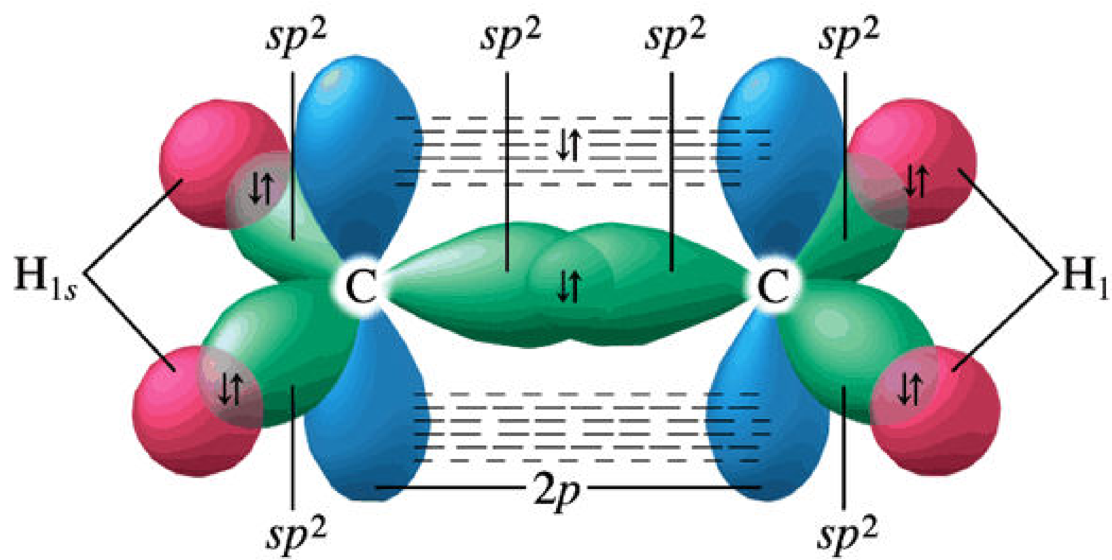


Pictorial views of the orbitals in ethylene



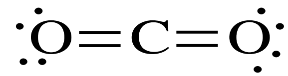




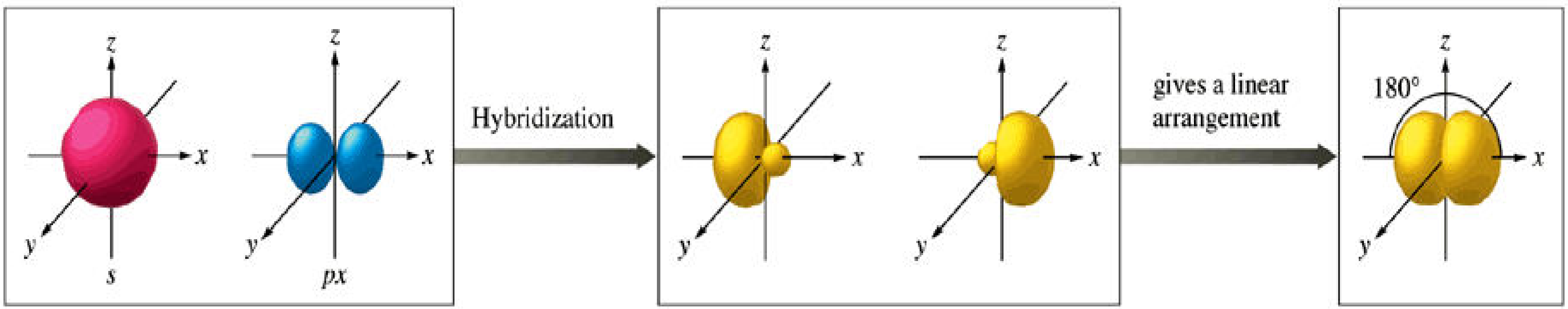


sp Hybridization: combination of an s orbital with an p orbitals to form two sp hybrid orbitals

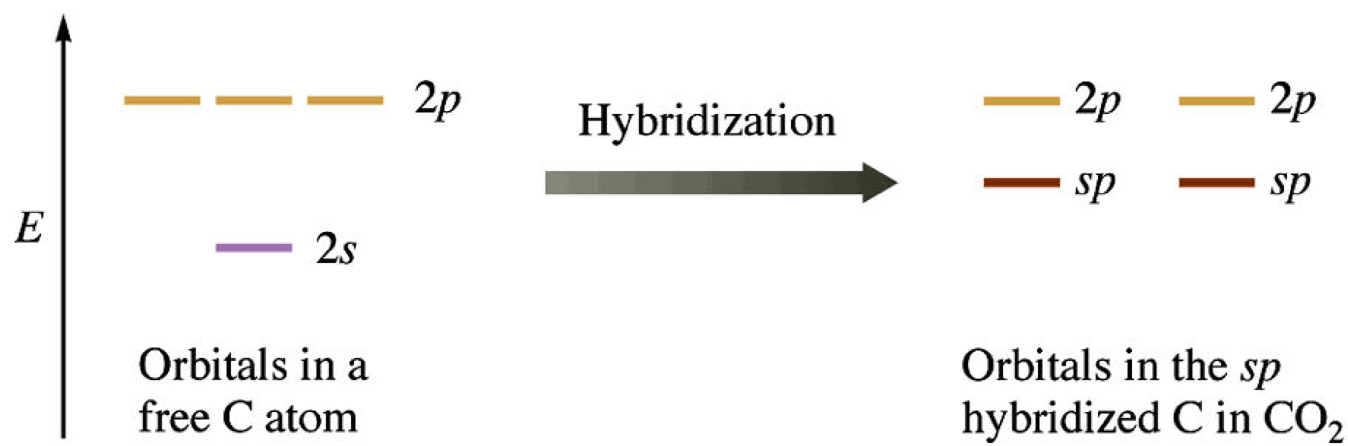
CO_2, carbon dioxide is our example



C atom uses 2s and one 2p orbital to make two sp hybrid orbitals that are 180 degrees apart

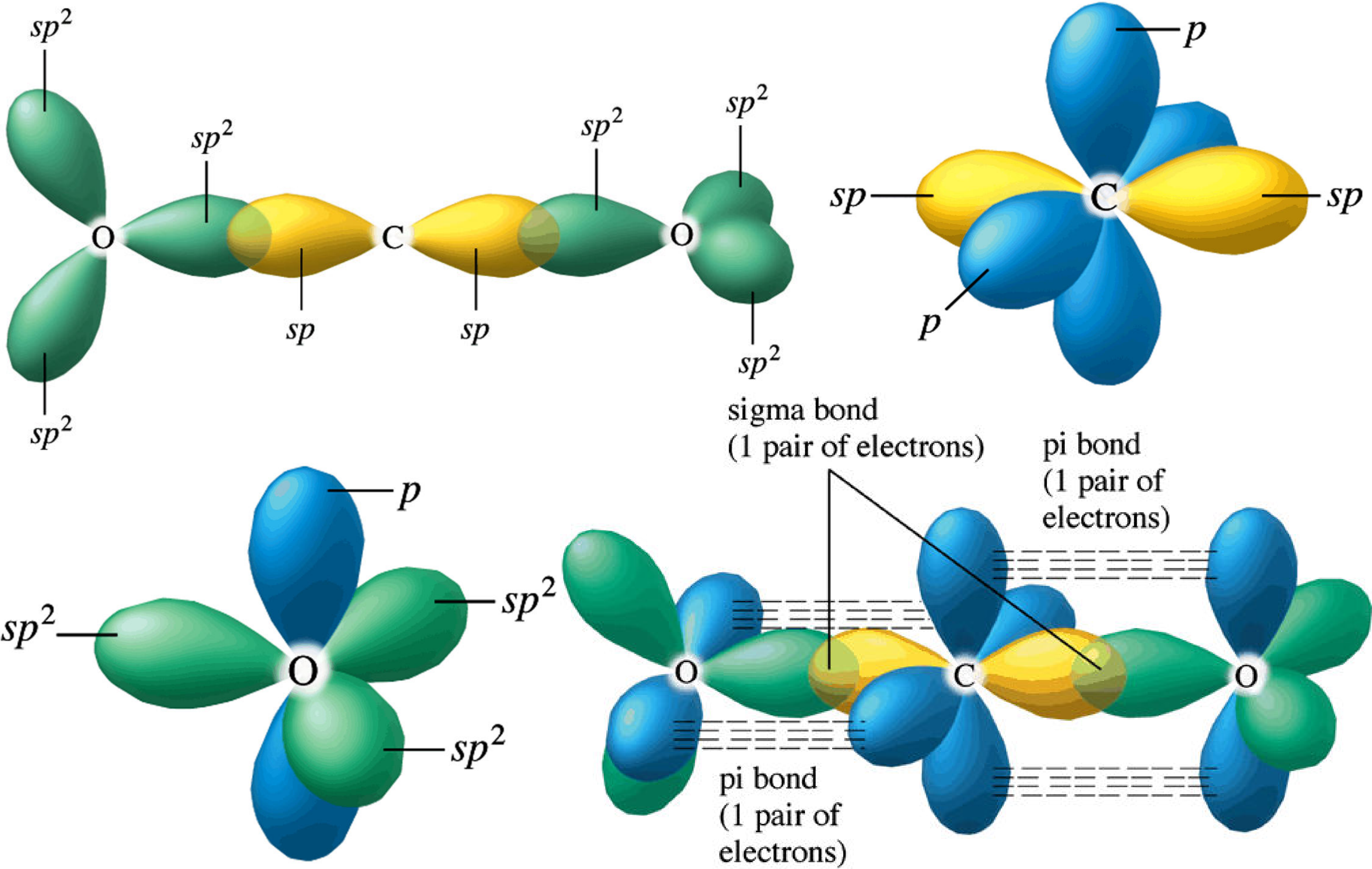


We get 2 degenerate sp orbitals and two unaltered 2p orbitals



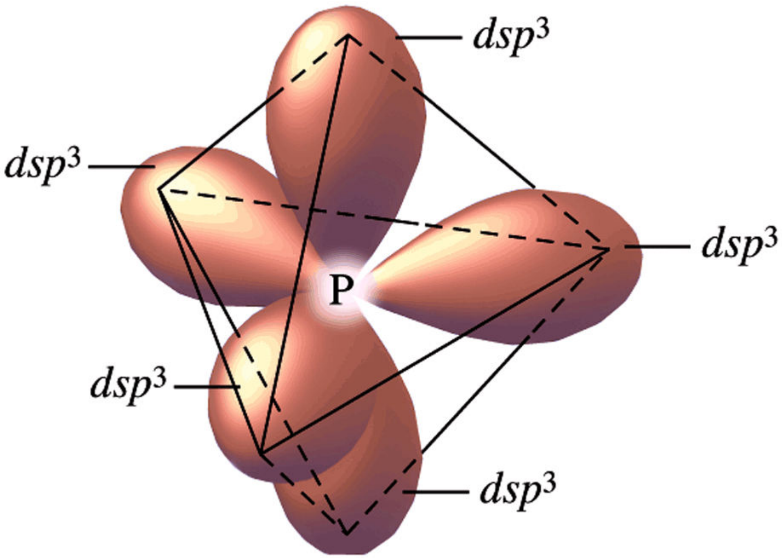
Oxygen uses sp^2 orbitals to overlap and form sigma bonds with C

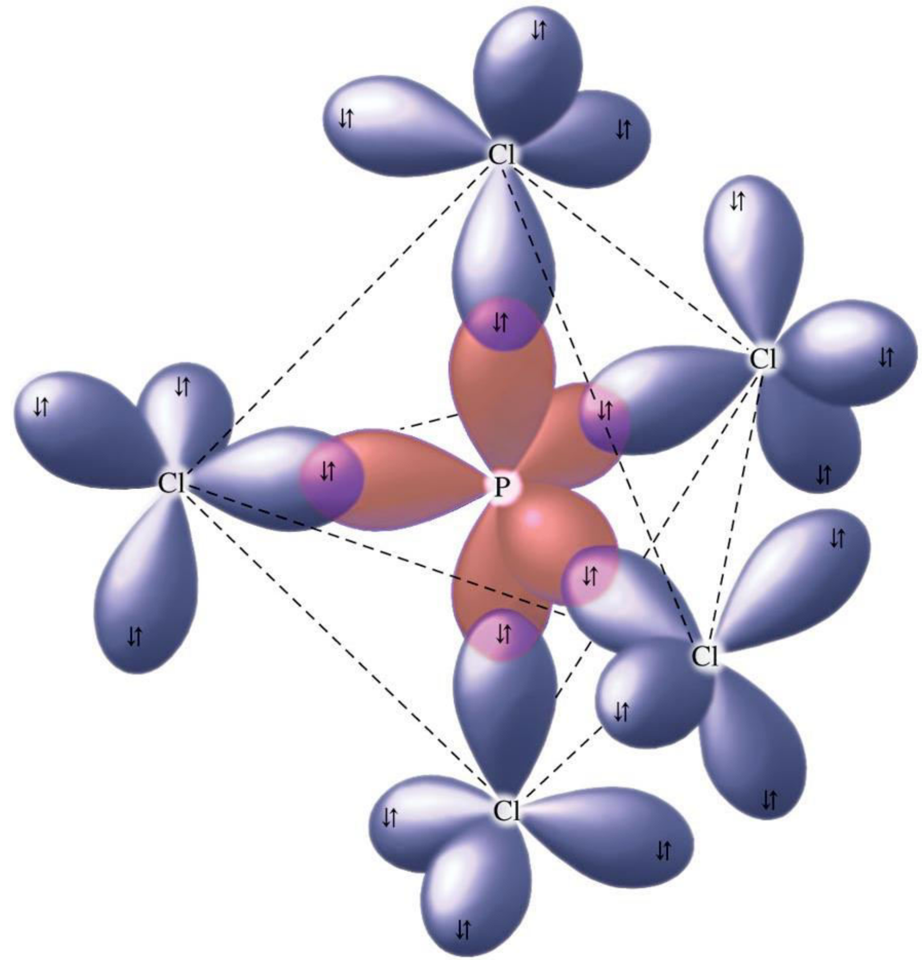
Free p orbitals on the O and C atoms form pi bonds to complete bonding



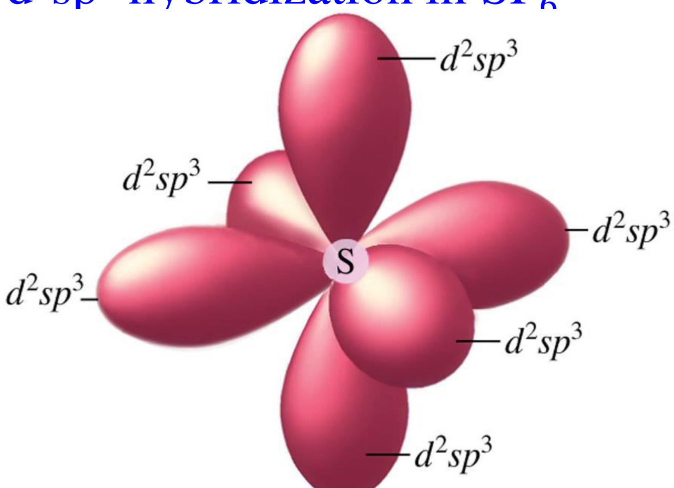
d-orbitals can also be involved in hybridization

1. dsp^3 hybridization in PCl_5

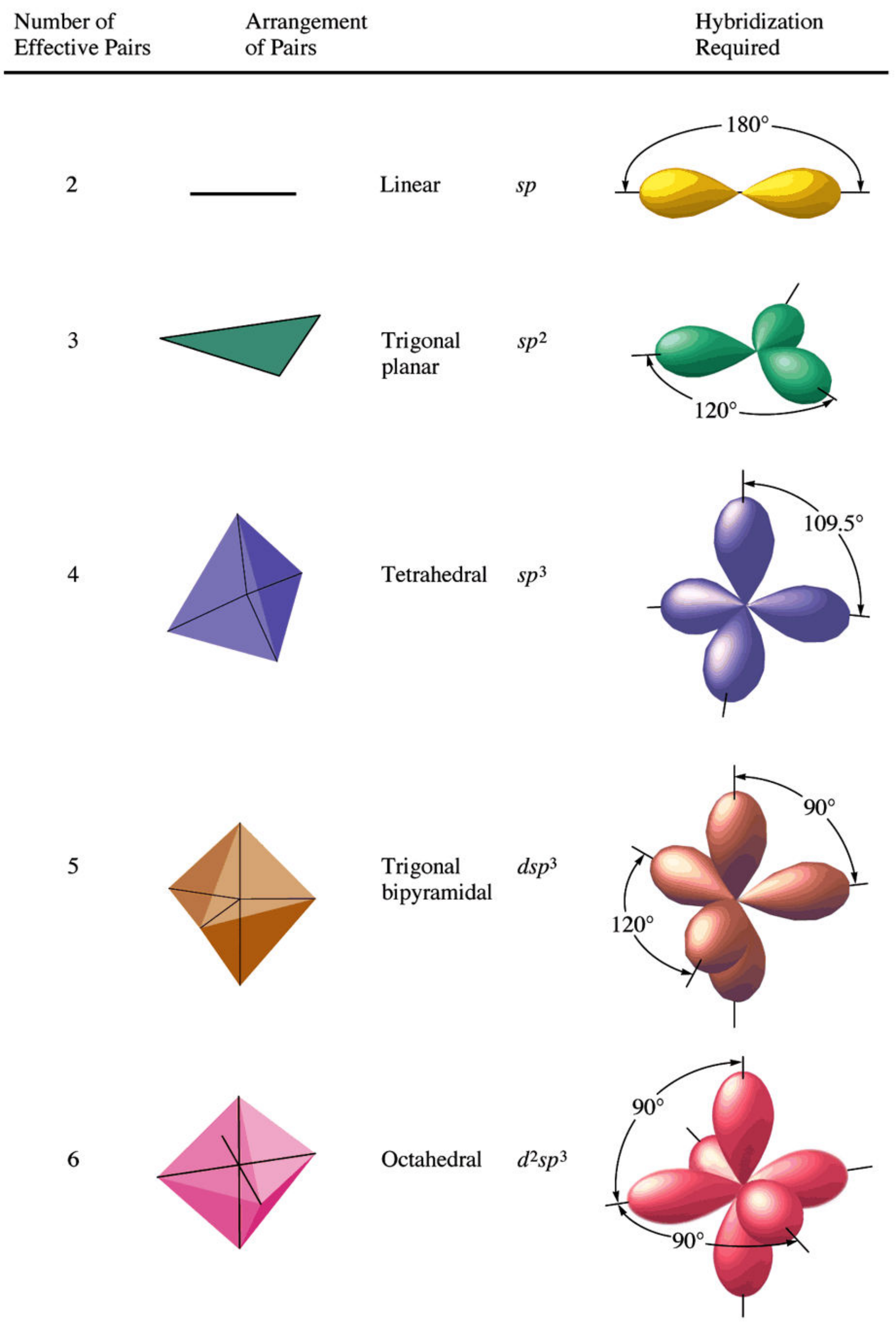




2. d^2sp^3 hybridization in SF_6



steric number	pure AOs s p d	hybrid AO	hybrid type	bond angles
2	1 1 0	2	sp	180°
3	1 2 0	3	sp2	120°
4	1 3 0	4	sp3	109.5°
5	1 3 1	5	sp^3d	90°,120°
6	1 3 2	6	sp^3d^2	90°



Sample Problems

Give the hybridization for the underlined atoms for the following molecules:

Caution! You must start with a good Lewis structure!

$\underline{N}H_2NH_2$

$CH_3\text{-}\underline{C}H{=}CH\text{-}CH_3$

$CH_3\text{-}CH{=}\underline{C}{=}CH\text{-}CH_3$

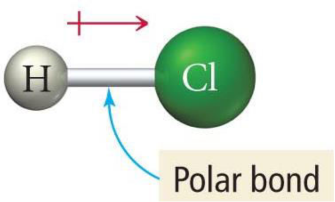
$H\underline{C}N$

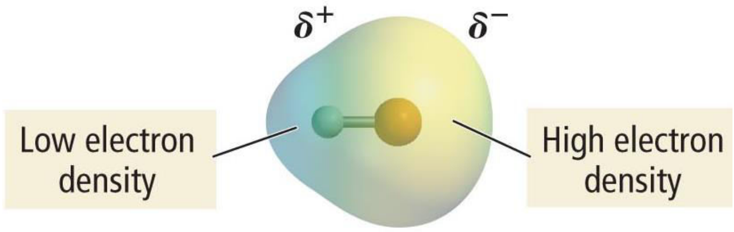
Polar Bonds and geometry of molecules

Any bond between atoms of different electronegativities is polar

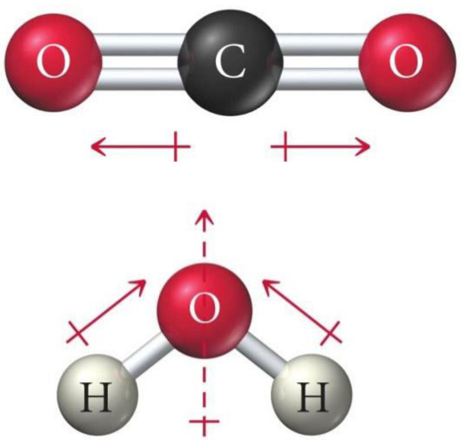
Electrons concentrate on one side of the bond

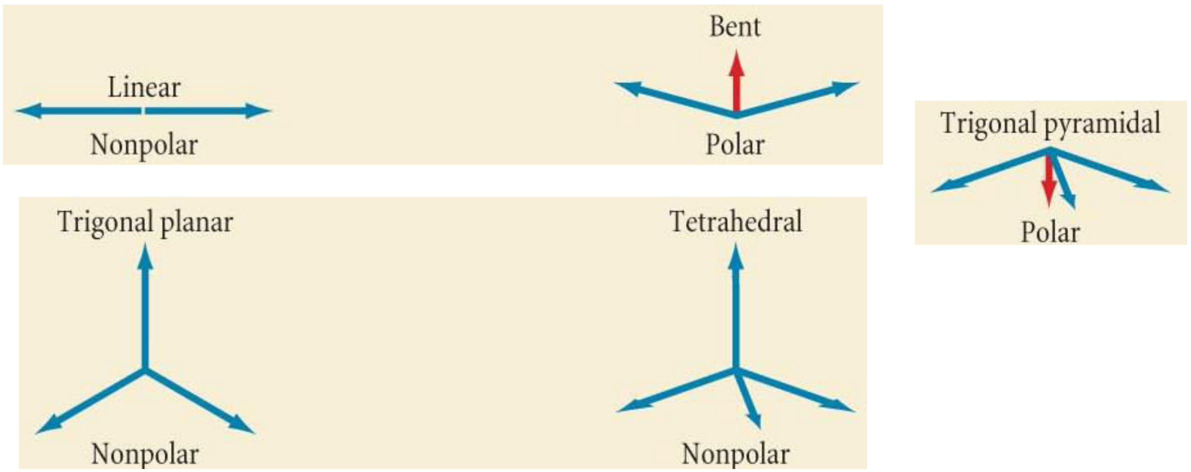
One end of the molecule is (+) and one end is (-)



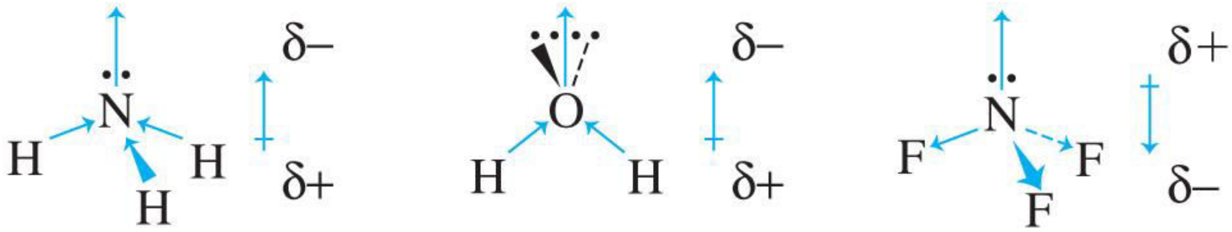


B. Complex molecules: vector addition of all bond dipoles

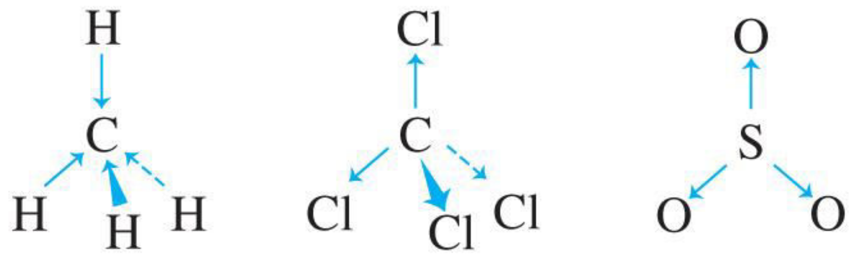




Examples:

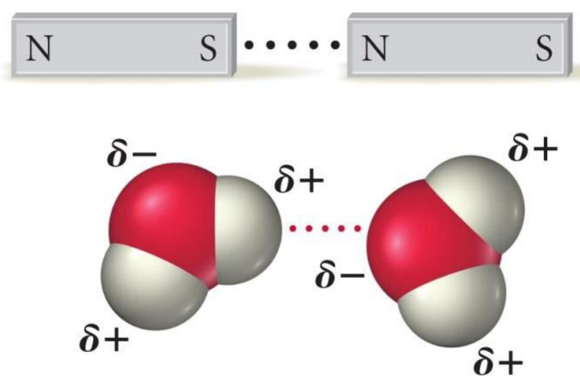


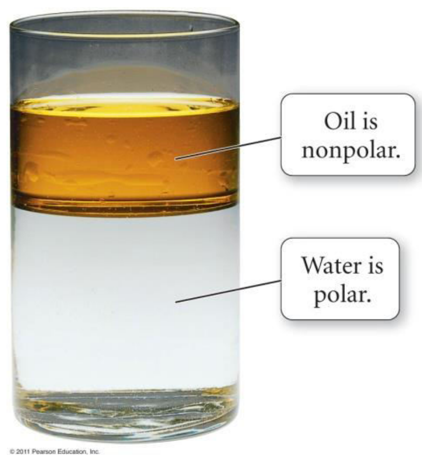
Net dipole, 1.47 D   Net dipole, 1.85 D   Net dipole, 0.23 D



Zero net dipole for all three

Polarity greatly affects molecular properties





Oppositely charged ends of polar molecules
Attract each other like opposite poles of magnets

Bond Dipole Moments

are due to differences in electronegativity.

depend on the amount of charge and distance of separation.

In debyes,

$\mu = 4.8 \ \text{x} \ \delta(\text{electron charge}) \ \text{x} \ d(\text{angstroms})$