



Quick Review

1. Drawing Lewis structures for organic compounds.
2. Drawing Lewis structures for covalent compounds that do not obey the octet rule.
3. VSEPR model.
4. We will not be talking about Molecular Orbital Model.

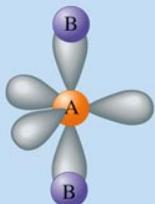
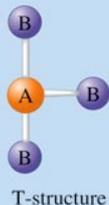
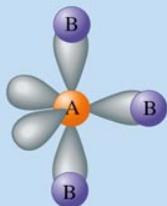
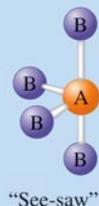
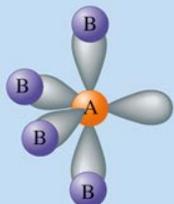
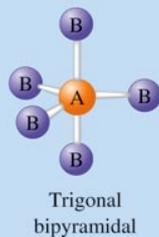
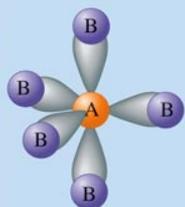
****HOUR EXAM II IS NEXT THURSDAY OCTOBER 30th at 7pm****



Trigonal Bipyramid Geometry

TABLE 8.8 Structures of Molecules with Five Electron Pairs Around the Central Atom

Electron-Pair Arrangement Molecular Structure



(a) Trigonal bipyramid shape: PCl_5

(b) See-saw shape: SF_4

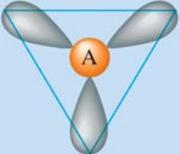
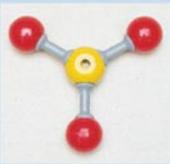
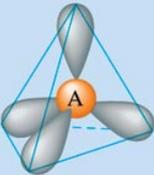
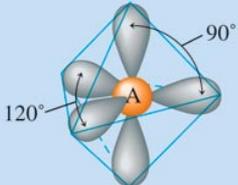
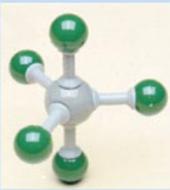
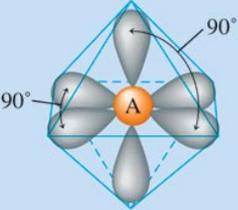
(c) T-shape: ICl_3

(d) Linear: KrF_2



Octahedral Geometry

TABLE 8.6 Arrangements of Electron Pairs Around an Atom Yielding Minimum Repulsion

| Number of Electron Pairs | Arrangement of Electron Pairs | Example |
|--------------------------|--|--|
| 2 | Linear  |  |
| 3 | Trigonal planar  |  |
| 4 | Tetrahedral  |  |
| 5 | Trigonal bipyramidal  |  |
| 6 | Octahedral  |  |

(a) Octahedral shape:
 SF_6

(b) Square pyramid shape:
 ICl_5

(c) Square planar shape:
 XeF_4



Bonding Orbitals

So far in our discussion of molecules we have focused on the arrangement of valence electrons.

We will now focus on bonding orbitals, the orbitals that hold valence electrons.

Example: H_2

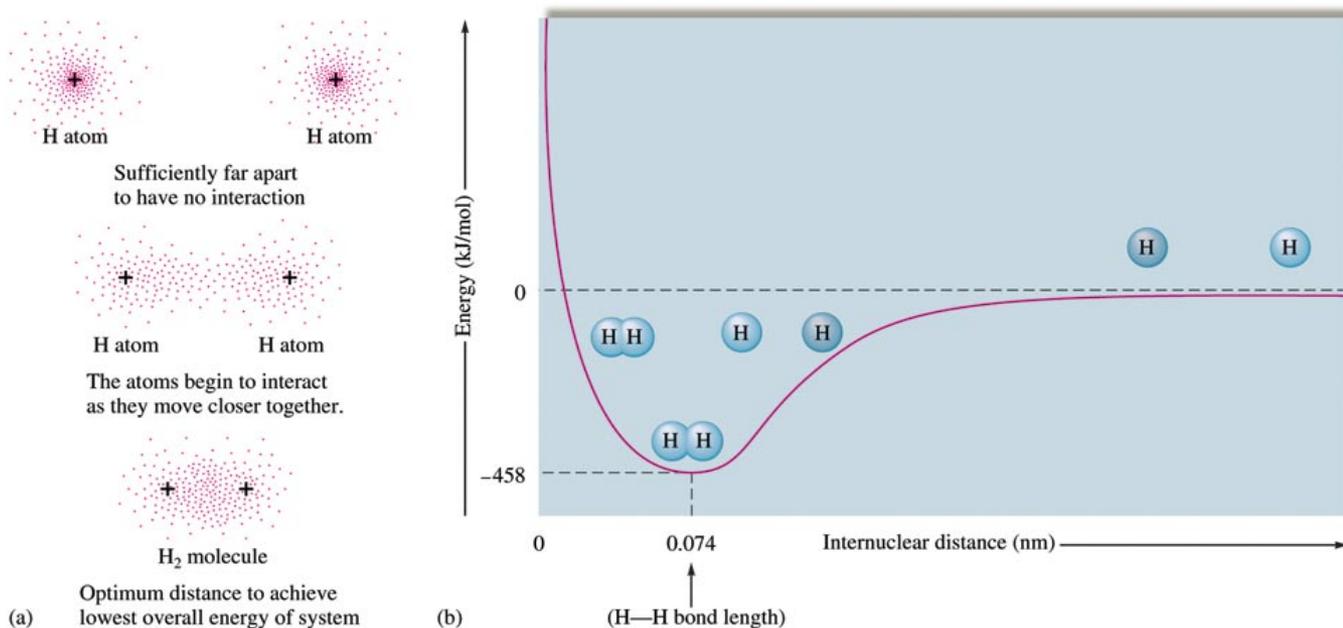


Bonding orbital represents on average where the two electrons in a bond reside.



Bonding Orbitals

Why does bonding represent a lower energy state?

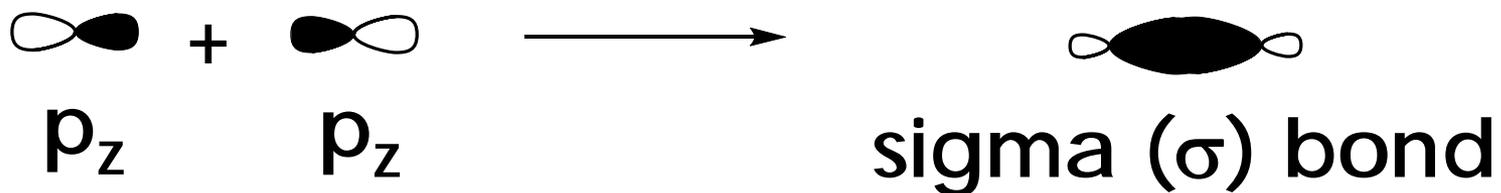


In separated atoms the valence electron is attracted to one nucleus whereas in H₂ the valence electrons are attracted to two nuclei.



Sigma Bonds

Example: $F_2 - 1s^2 2s^2 2p^5$



Electron density is on the internuclear axis.

End-end or head to head overlap of orbitals, for example, $p_z + p_z$ or $1s + 1s$ as in H_2 .

Sigma orbitals can be rotated without breaking the bond since orbitals still overlap upon rotation.



Pi Bonds

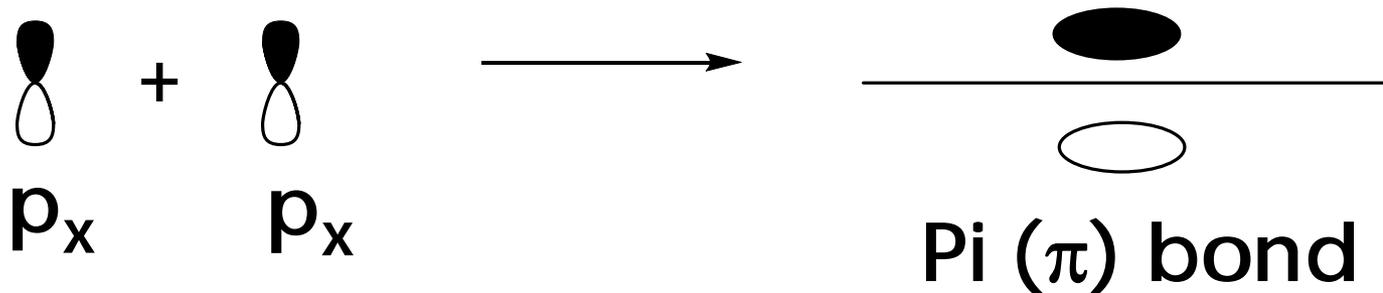
Example: $O_2 - 1s^2 2s^2 2p^4$

Must account for two bonds.

Assume z axis is the internuclear axis.

The two $2p_z$ orbitals overlap to form a sigma bond.

The second bond is formed from side-side overlap of p_x orbitals.



Electron density is above and below the internuclear axis.
Pi bonds can't be rotated without disrupting the orbital overlap.



Multiple Bonds

In general:

A single bond is composed of a sigma bond.

A double bond is composed of a sigma bond + 1 pi bond.

A triple bond is composed of a sigma bond + 2 pi bonds.

Example: $\text{N}_2 - 1s^2 2s^2 2p^3$

3 bonds to account for.

Two $2p_z$ orbitals overlap to form a sigma bond.

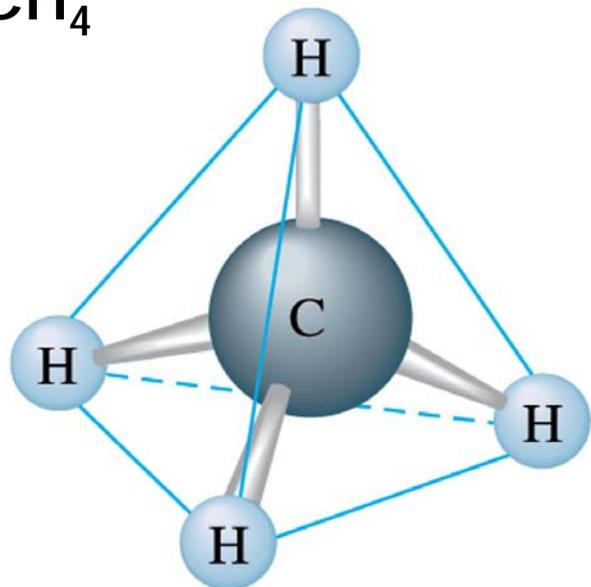
Two $2p_y$ orbitals overlap to form a pi bond.

Two $2p_x$ orbitals overlap to form another pi bond.



More Complicated Bonding Motifs

CH₄



What is the geometry and shape of this molecule?

What are the bond angles about the central atom?

Simple overlap of atomic orbitals can't explain the 109.5° bond angles of methane.

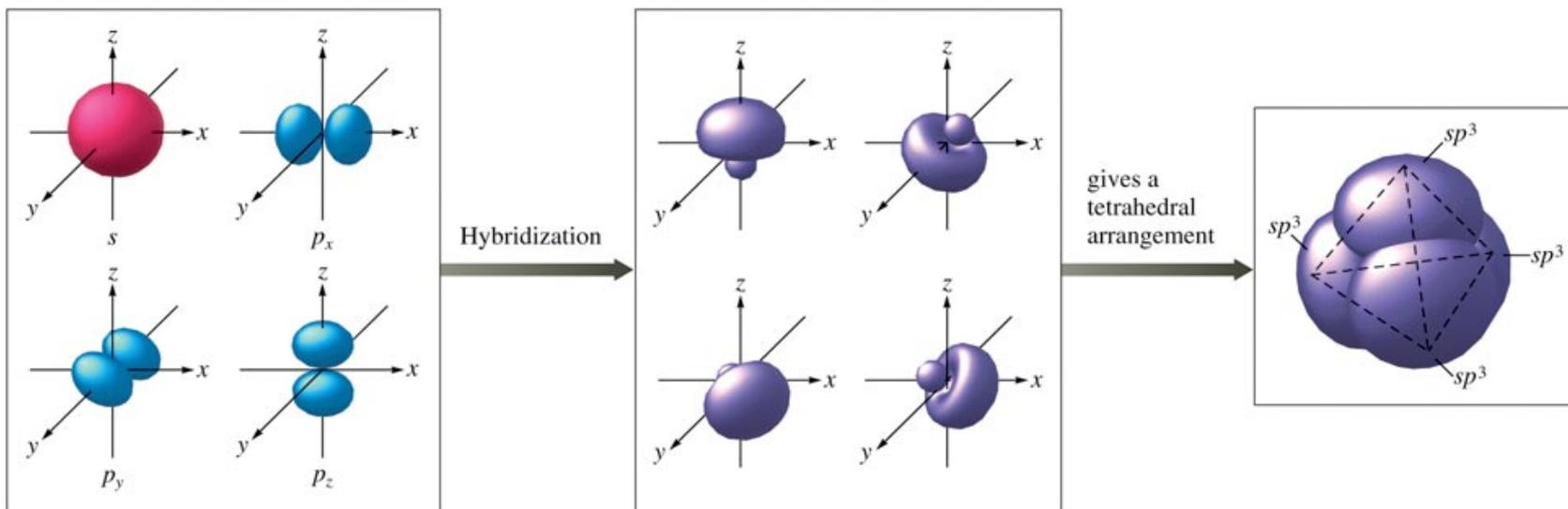
If *s*, *p*, *d*, *f* orbitals overlapped to form all bonds then all bond angles would be 90 and 180° but this is NOT the case.



Hybrid Orbitals

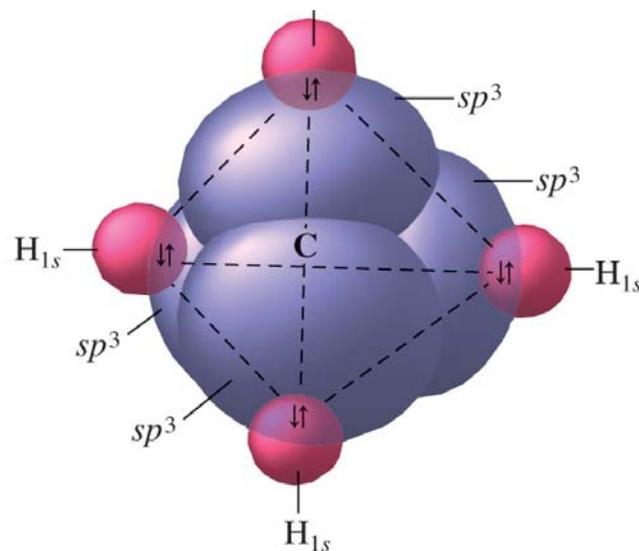
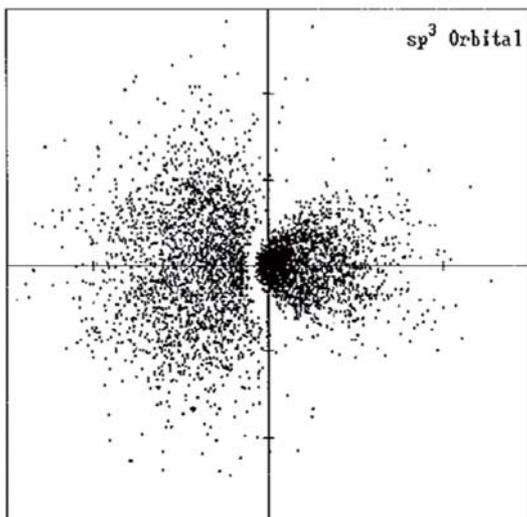
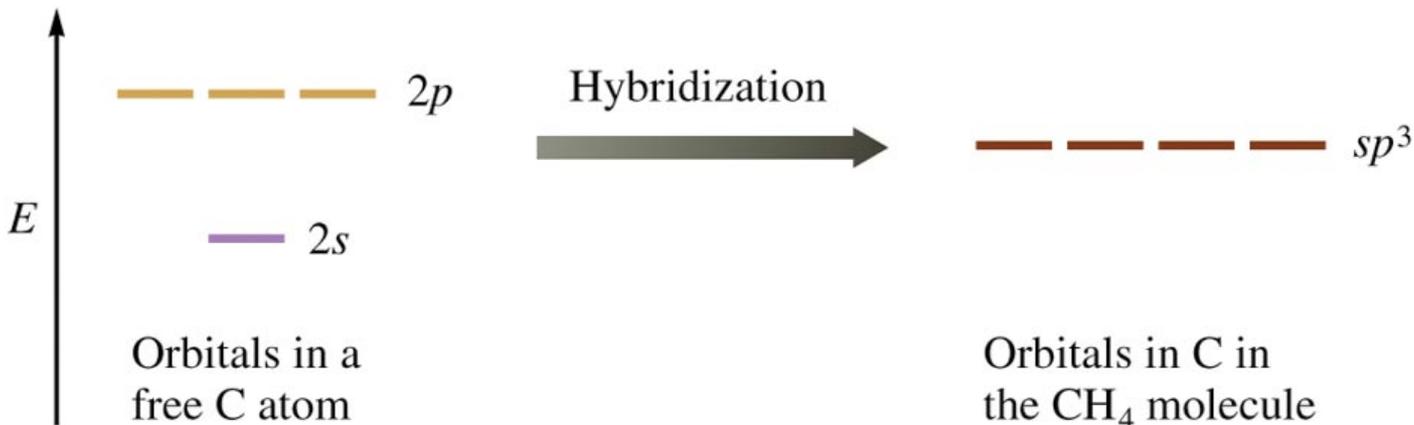
Hybrid Orbitals – used to explain the geometry seen in polyatomic molecules. Hybridization involves the mixing of atomic orbitals.

For CH_4 we combine the carbon 2s and three carbon 2p orbitals to result in four hybrid sp^3 orbitals.





sp^3 Hybrid Orbitals

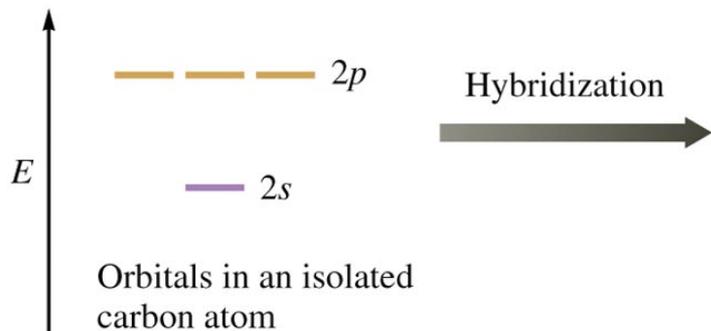


Tetrahedral geometry = sp^3 hybridization

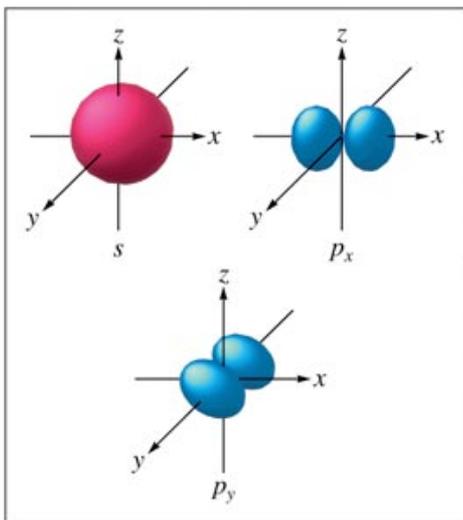
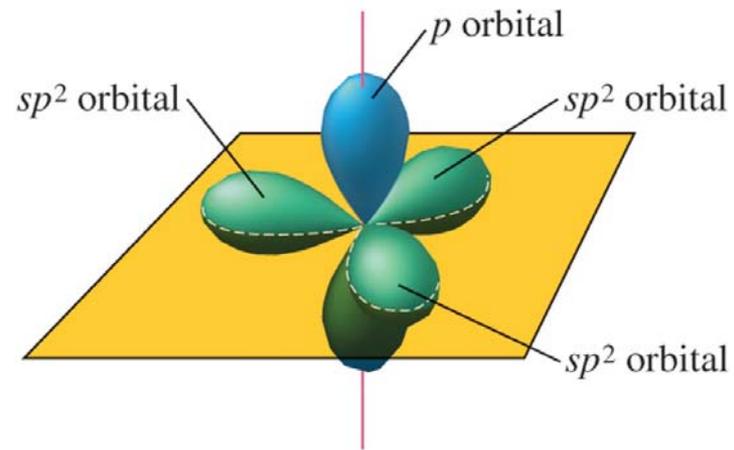
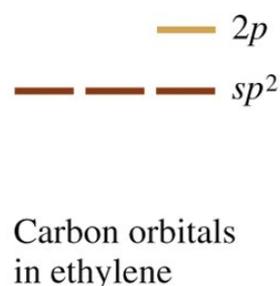


sp^2 Hybrid Orbitals

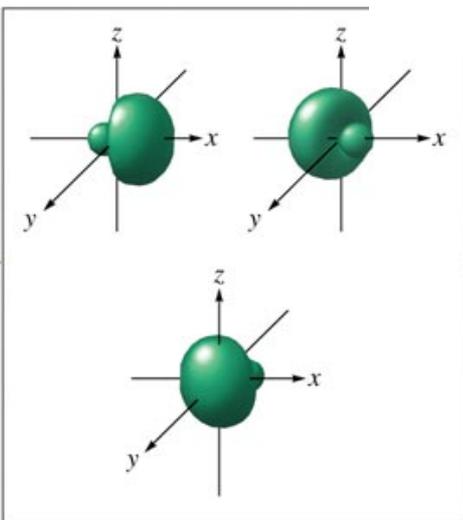
Example: C_2H_4



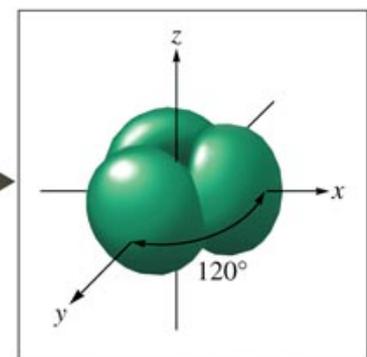
Hybridization



Hybridization

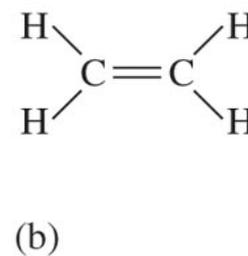
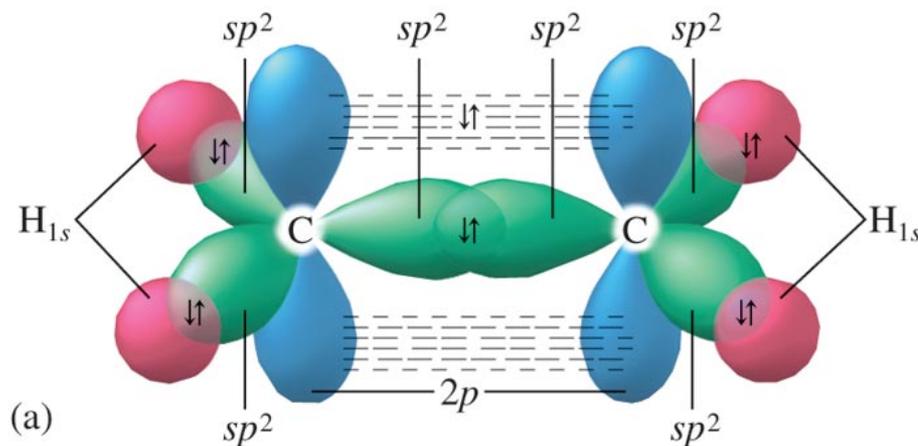
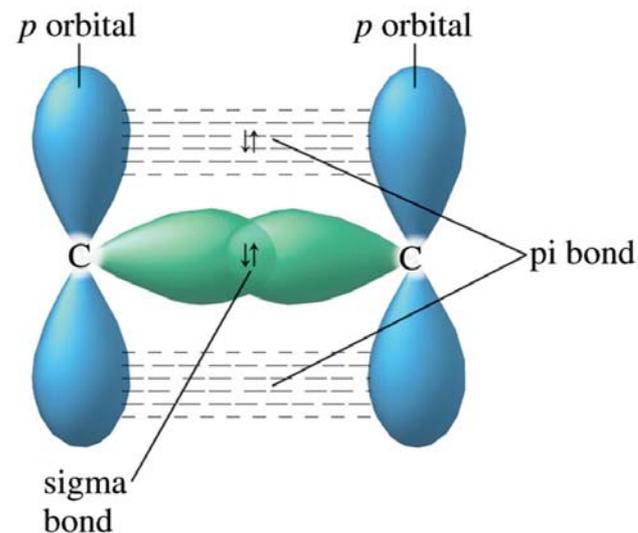
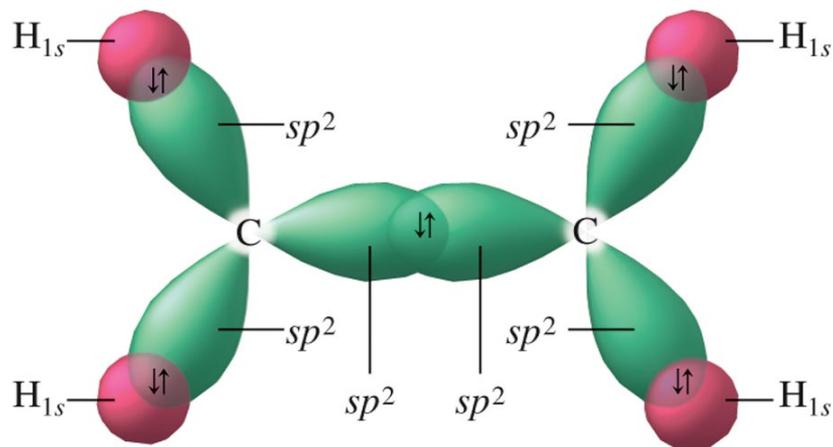


gives a trigonal planar arrangement





sp^2 Hybrid Orbitals

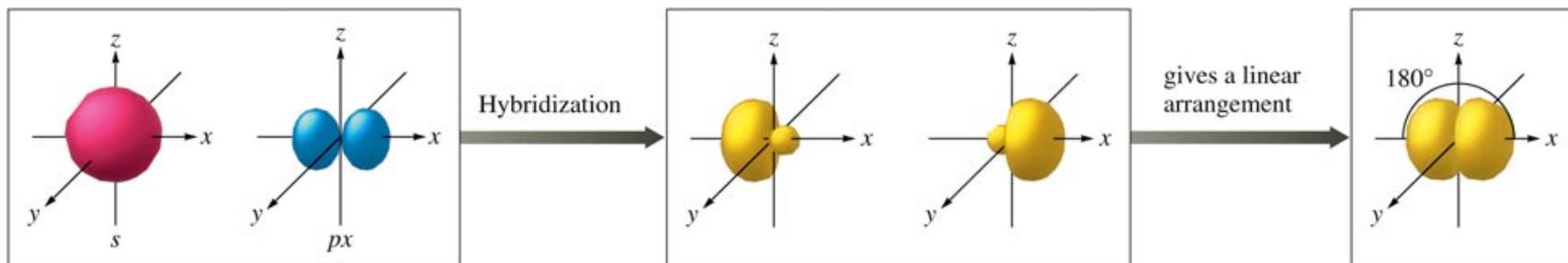
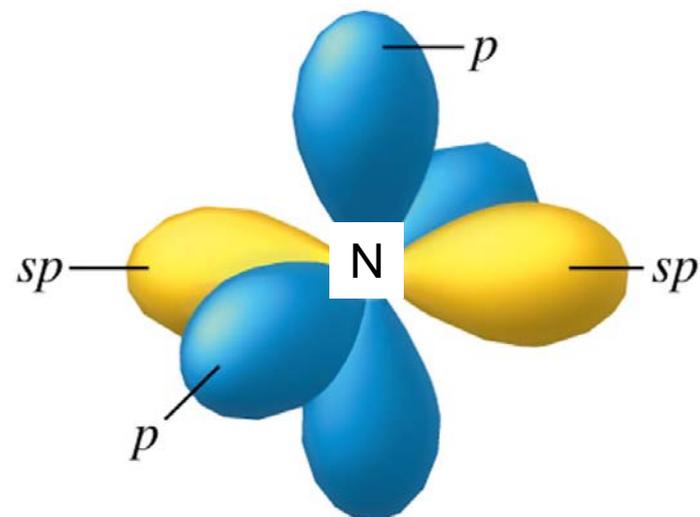
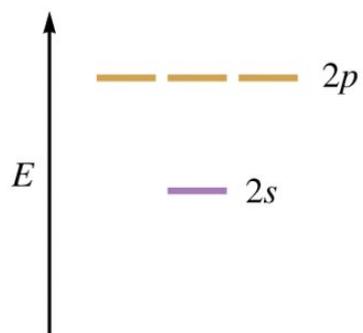


Trigonal planar geometry = sp^2 hybridization



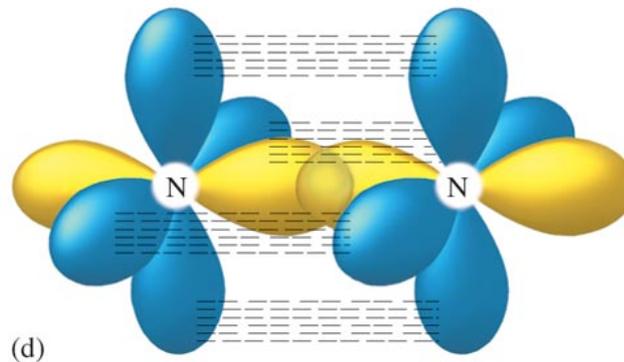
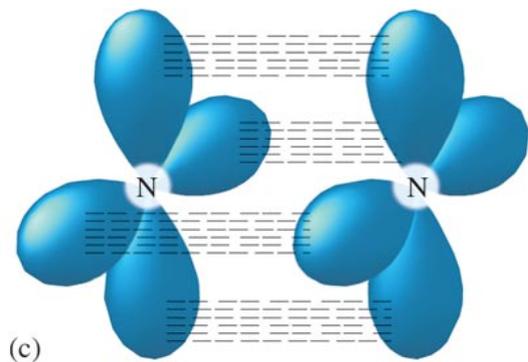
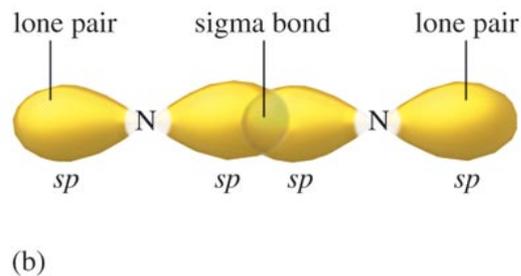
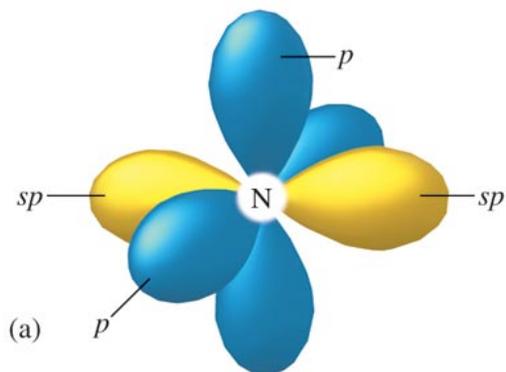
sp Hybrid Orbitals

Example: N₂





sp Hybrid Orbitals



Linear geometry = sp hybridization

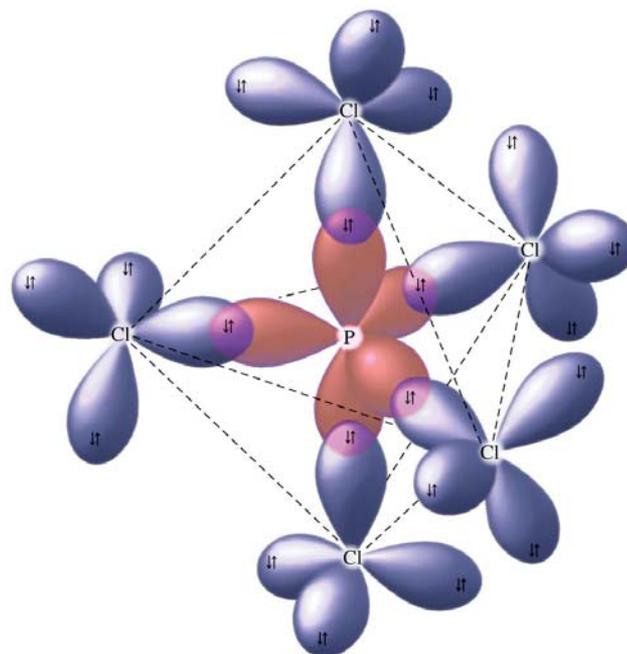
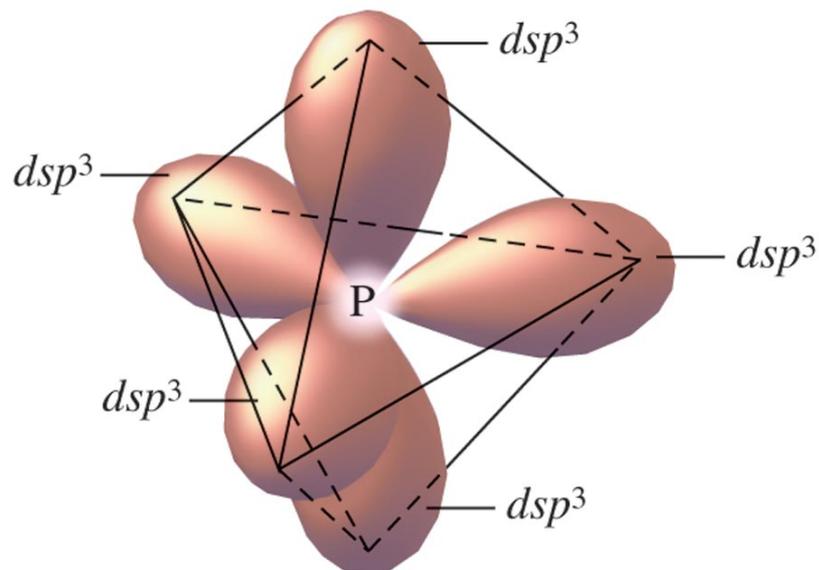


dsp^3 Hybrid Orbitals

For molecules with trigonal bipyramidal geometry:

$$d + s + 3xp = 5 \text{ } dsp^3 \text{ hybrids}$$

Example: PCl_5



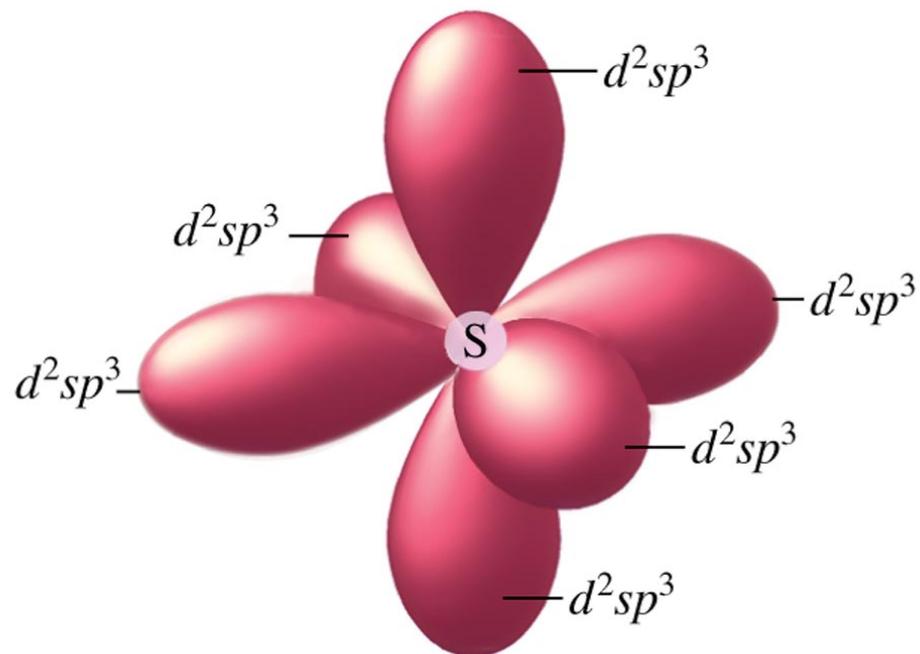


d^2sp^3 Hybrid Orbitals

For molecules with octahedral geometry:

$$2x d + s + 3xp = 6 d^2sp^3 \text{ hybrids}$$

Example: SF_6





Summary

| Number of Effective Pairs | Arrangement of Pairs | | Hybridization Required | |
|---------------------------|----------------------|----------------------|------------------------|--|
| 2 | | Linear | sp | |
| 3 | | Trigonal planar | sp^2 | |
| 4 | | Tetrahedral | sp^3 | |
| 5 | | Trigonal bipyramidal | dsp^3 | |
| 6 | | Octahedral | d^2sp^3 | |

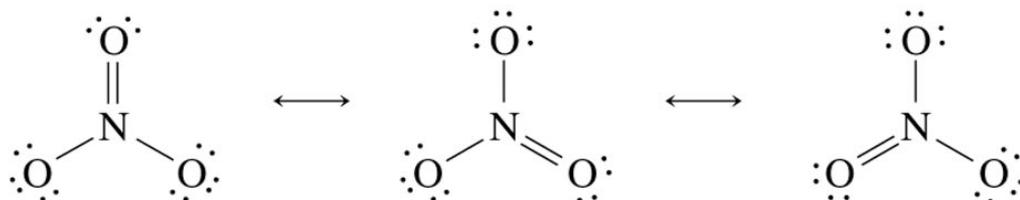
What you need to be able to do:

1. Know how to predict hybridization around central atom.
2. Know difference between sigma and pi bonds.
3. Be able to count the number of sigma and pi bonds in a molecule.
4. Be able to predict which orbitals overlap to form sigma and pi bonds.

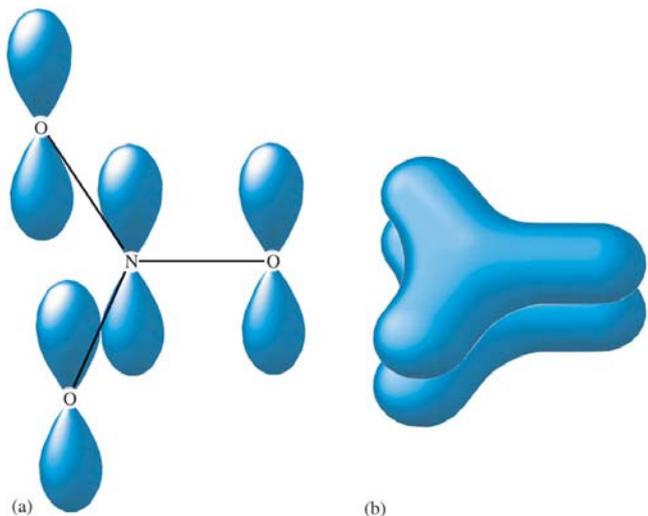


Delocalization

Example: NO_3^-



Experiment tells us that N-O bond lengths are equal in length.



Explained by stating that the pi electrons are delocalized over the entire surface of the molecule.

Extra stability the more resonance structures can be drawn because delocalization helps to minimize electron-electron repulsions.



Delocalization

Example: C_6H_6 (benzene)

