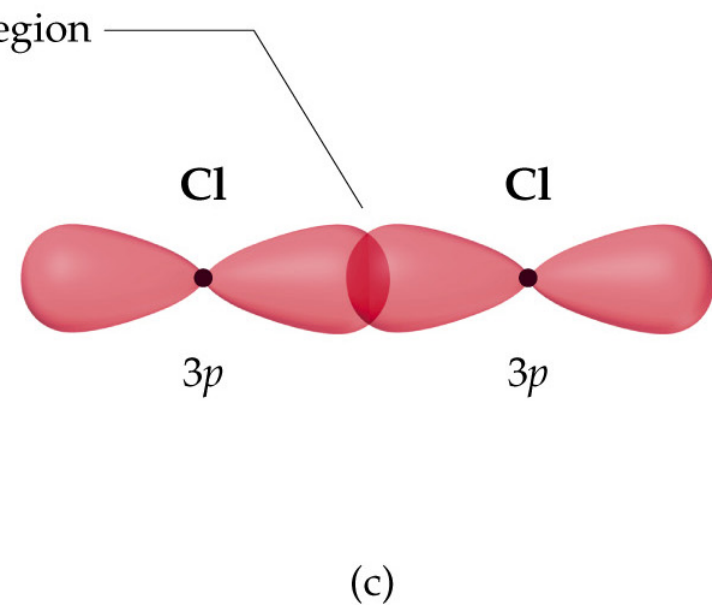
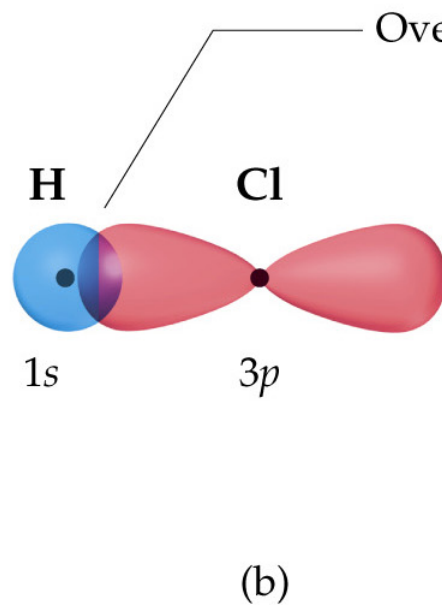
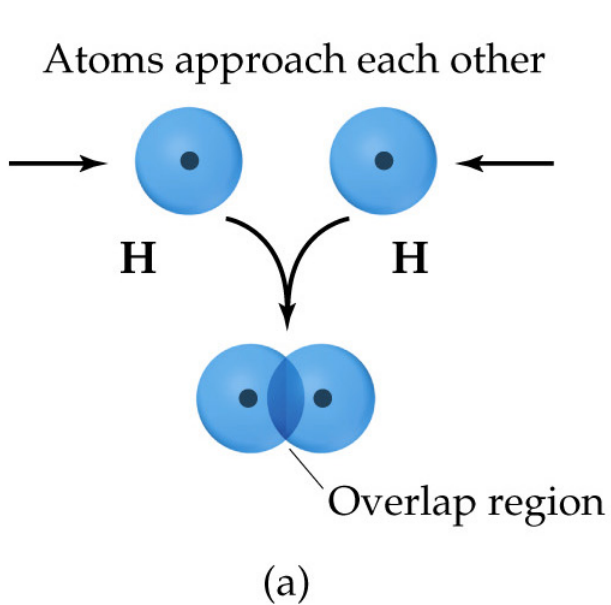


Combining Lewis Structures and VSEPR with atomic orbitals

Covalent Bonding and Orbital Overlap

- **Lewis structures and VSEPR do not explain why a bond forms.**
- **How do we account for shape in terms of quantum mechanics?**
- **What are the orbitals that are involved in bonding?**
- **We use Valence Bond Theory:**
 - **Bonds form when orbitals on atoms overlap.**
 - **There are two electrons of opposite spin in the orbital overlap.**



s-orbitals are spherical.

p_x , p_z , and p_y are perpendicular to each other. 180° and 90° bond angle could be explained by overlap of p-orbitals but 120° and 109.5° could not

Hybridization Model

- There is a model to explain the shape of molecules using atomic orbitals mixing.
- Atomic orbitals can mix or hybridize in order to adopt an appropriate geometry for bonding.
- Hybridization is determined by the electron domain geometry.

Hybrid Orbitals

sp Hybrid Orbitals

Consider the BeF_2 molecule (experimentally known to exist):

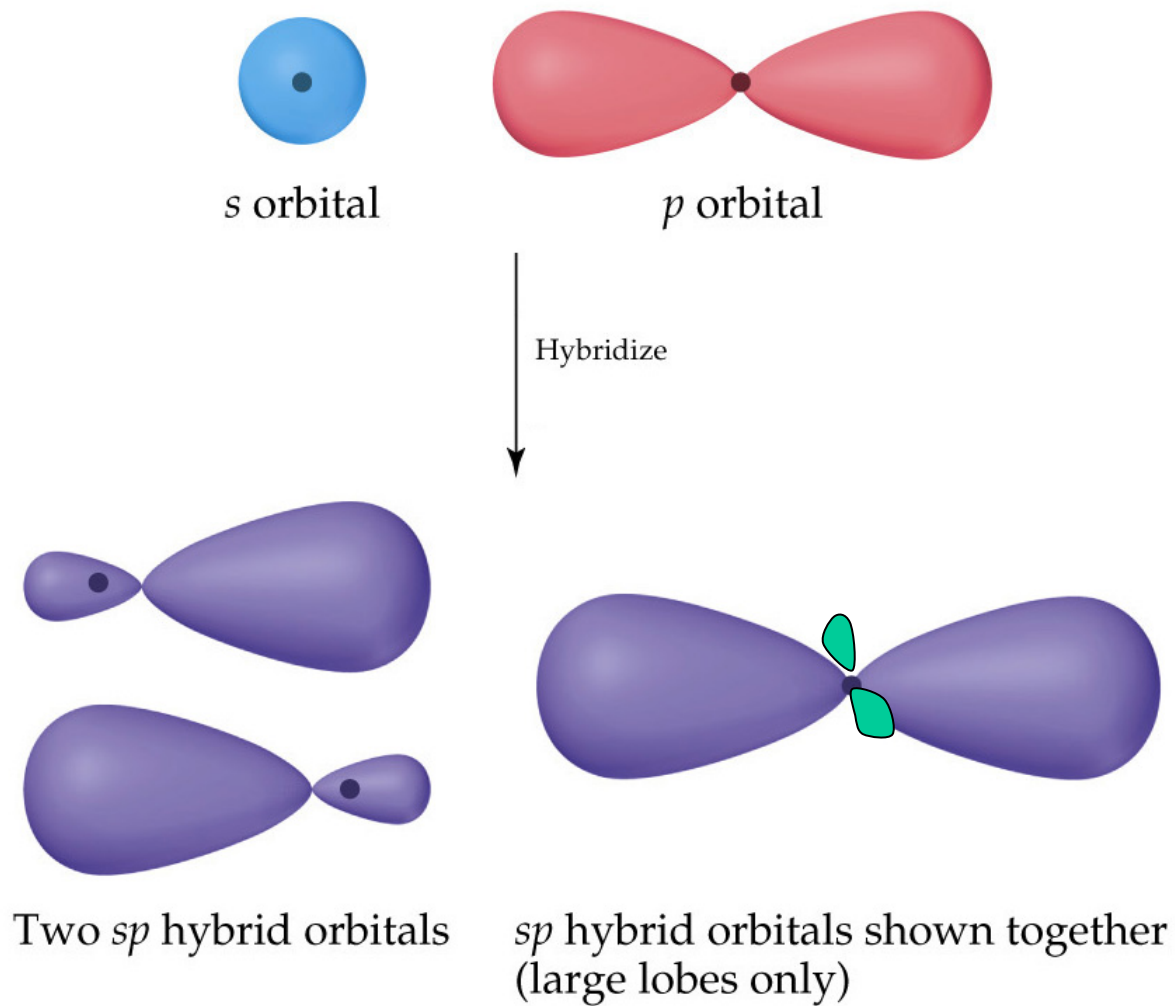
Be has a $1s^2 2s^2$ electron configuration.

- There is no unpaired electron available for bonding.
- We conclude that the atomic orbitals are not adequate to describe orbitals in molecules.
- We know that the F-Be-F bond angle is 180° (VSEPR theory).
- We also know that one electron from Be is shared with each one of the unpaired electrons from F.

- **We assume that the Be orbitals in the Be-F bond are 180° apart.**
 - **We could promote an electron from the 2s orbital on Be to the 2p orbital to get two unpaired electrons for bonding.**
 - **BUT the geometry is still not explained.**
- **We can solve the problem by allowing the 2s and one 2p orbital on Be to mix or form a hybrid orbital..**
- **The hybrid orbital comes from an s and a p orbital and is called an sp hybrid orbital.**

sp Hybrid Orbitals

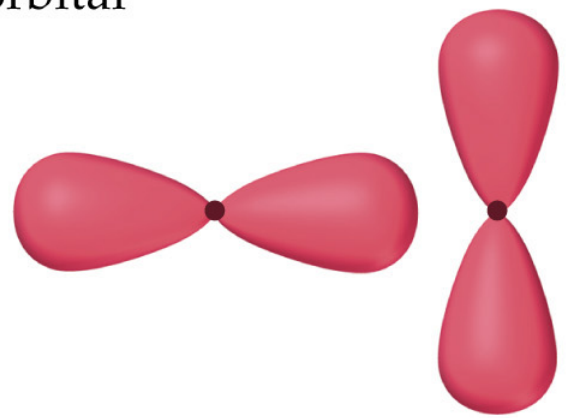
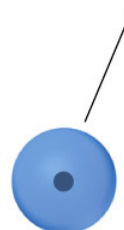
- The lobes of sp hybrid orbitals are 180° apart.



sp^2 Hybrid Orbitals

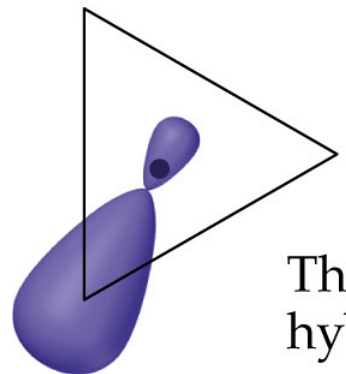
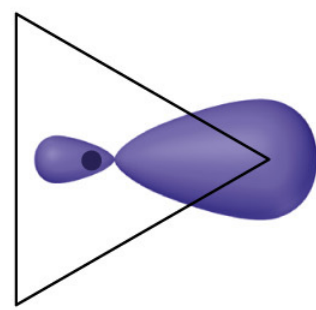
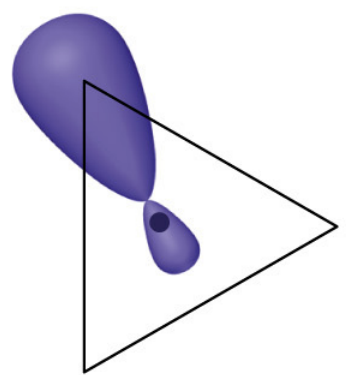
- ***Important:*** when we mix n atomic orbitals we must get n hybrid orbitals.
- sp^2 hybrid orbitals are formed with one s and two p orbitals. (Therefore, there is one unhybridized p orbital remaining.)
- The large lobes of sp^2 hybrids lie in a trigonal plane.
- All molecules with trigonal planar electron pair geometries have sp^2 orbitals on the central atom.

One s orbital



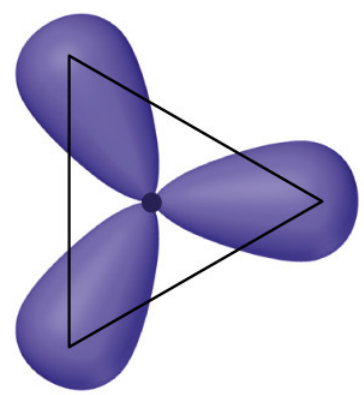
Two p orbitals

Hybridize



Three sp^2 hybrid orbitals

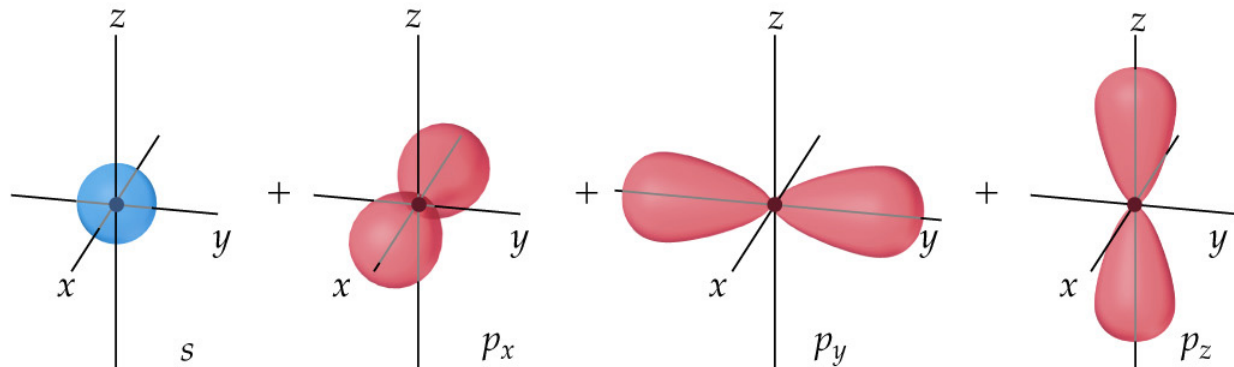
sp^2 hybrid orbitals shown together (large lobes only)



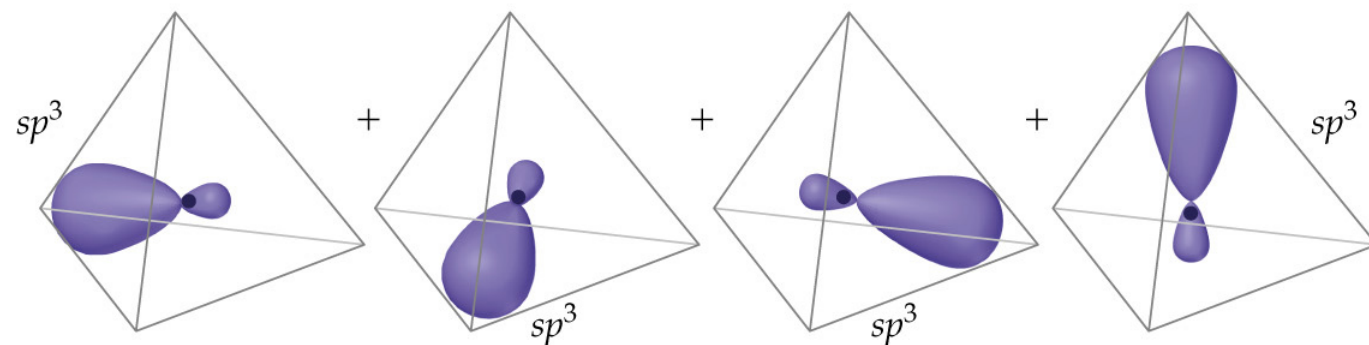
sp^3 Hybrid Orbitals

- sp^3 Hybrid orbitals are formed from one s and three p orbitals. Therefore, there are four large lobes.
- Each lobe points towards the vertex of a tetrahedron.
- The angle between the large lobes is 109.5° .
- All molecules with tetrahedral electron pair geometries are sp^3 hybridized.

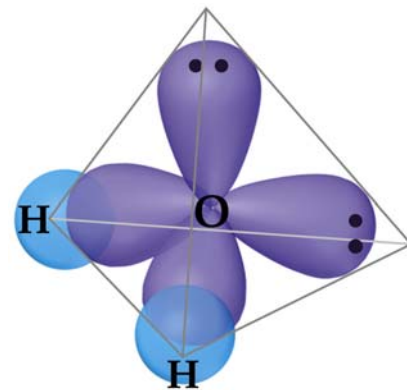
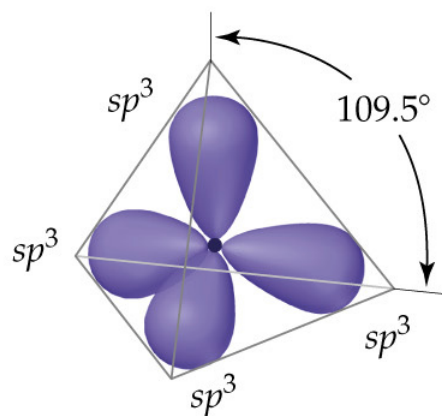
sp^3 Hybrid Orbitals



Hybridize to form four sp^3 hybrid orbitals



Shown together (large lobes only)

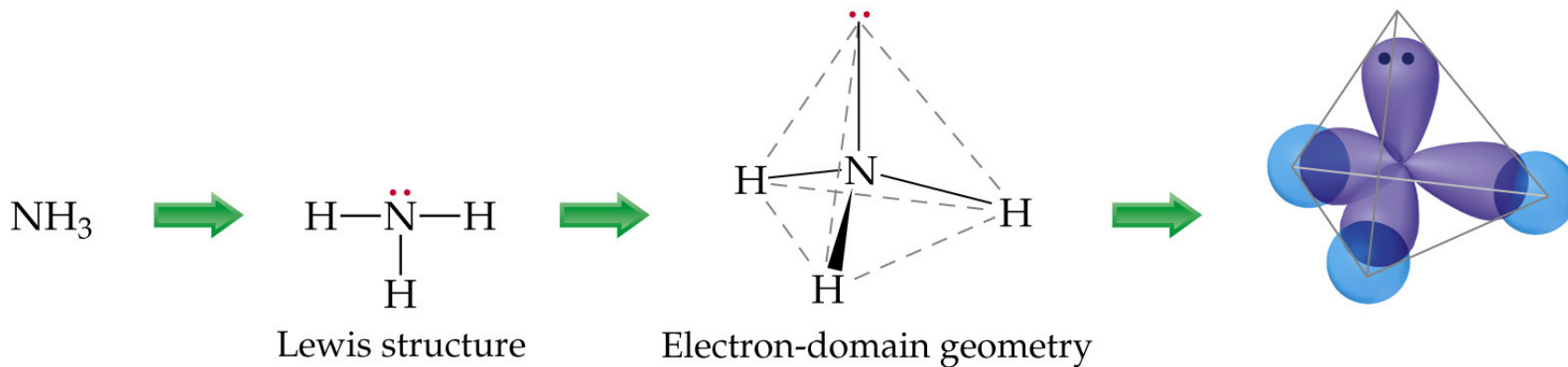


Hybridization Involving d Orbitals

- Since there are only three p -orbitals, trigonal bipyramidal and octahedral electron domain geometries must involve d -orbitals.
- Trigonal bipyramidal electron domain geometries require sp^3d hybridization.
- Octahedral electron domain geometries require sp^3d^2 hybridization.
- Note the electron domain geometry from VSEPR theory determines the hybridization.

Summary

1. Draw the Lewis structure.
2. Determine the electron domain geometry with VSEPR.
3. Specify the hybrid orbitals required for the electron pairs based on the electron domain geometry.



Deviations from the ideal bond angles: partial hybridization

$sp >$	$sp^2 >$	$sp^3 >$	p
180	120	109.5	90

The greater the s-contribution the greater the bond angle

H₂O: 104.5 ????

Hybridization index, n

$$1+n \cos\theta = 0$$

$$n = -1/\cos \theta = -1/\cos 104.5 = -1/(-0.250) = 4$$

Hybridization for water is sp^4

It does not mean that there are 4 p-orbitals!

it means that each hybrid consists of 20% of s and 80% of p AOs

More p-character at the O-H bonds and more s-character for lone pairs

A combination of partial hybridization with **electronegativities** has predictive power