

Today's Class

Hybridization

Hybridization Theory

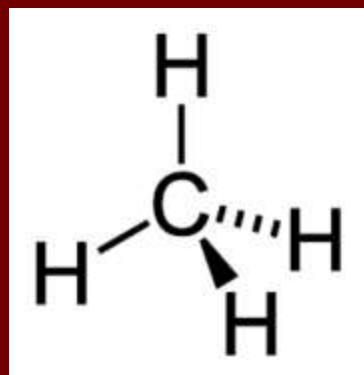
- **Used to explain some of the shapes of molecules in VSEPR Theory**
- **Hybridization Theory says that atoms bonded molecules will undergo structural changes in their valence level atomic orbitals.**
- **The atomic orbitals are converted into a new set of orbitals called Hybrid Orbitals.**
- **The Hybrid Orbitals will have some characteristics of the original atomic orbitals, but differ somewhat in shape**

Hybridization Theory

- In biology, the word "hybrid" usually refers to a genetic mixing.
- Hybridization: process of combining two or more atomic orbitals to create new orbitals(hybrids) that explain the geometry of the compound
- When determining the types of hybrid orbitals that an atom has, you must first determine the number of groups around that atom much like VSEPR theory
- For basic hybridization theory, atoms will generally be surrounded by two, three, or four groups of electrons.

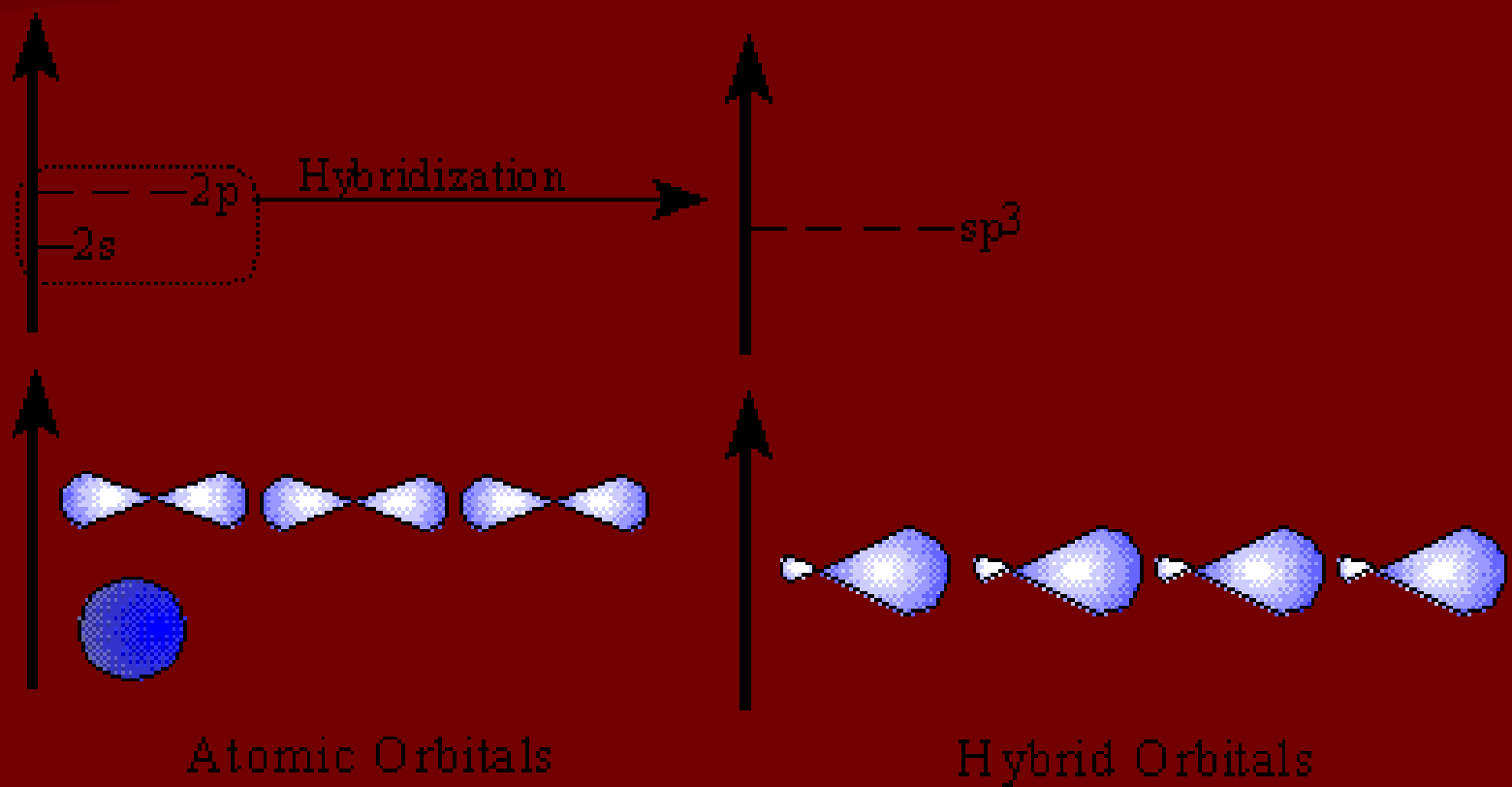
sp^3 hybridized

- Consider Methane(CH_4)- Has tetrahedral shape- six bond angles between the Hydrogens and the central Carbon where the angles are all 109.5°
- Experimental information has shown that all four bonds in this structure are identical, implying that they are made in exactly the same way.

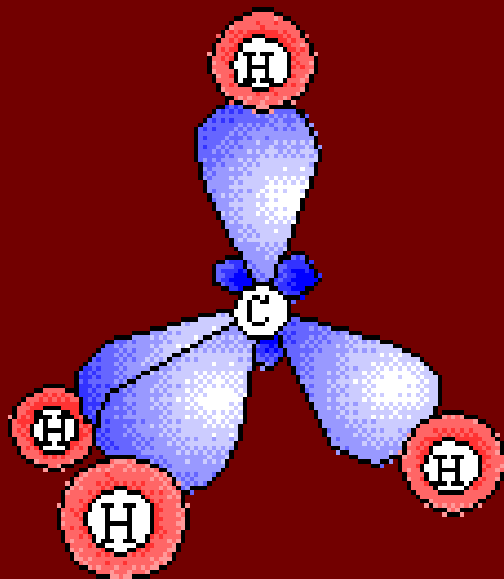


sp^3 hybridized

- In order to produce four identical orbitals it is necessary to hybridize four atomic orbitals. The Carbon atom has four valence atomic orbitals, one s orbital and three p orbitals. When these orbitals are hybridized, they will produce four identical hybrid orbitals
- The hybrids will consist of 75% p character and 25% s character so they should look much more like p orbitals than s orbitals.
- The new orbitals are called sp^3 hybrids. Shown on the next slide



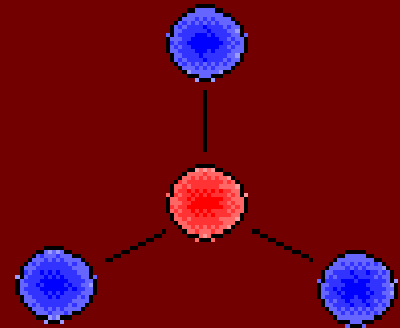
sp^3 hybridized

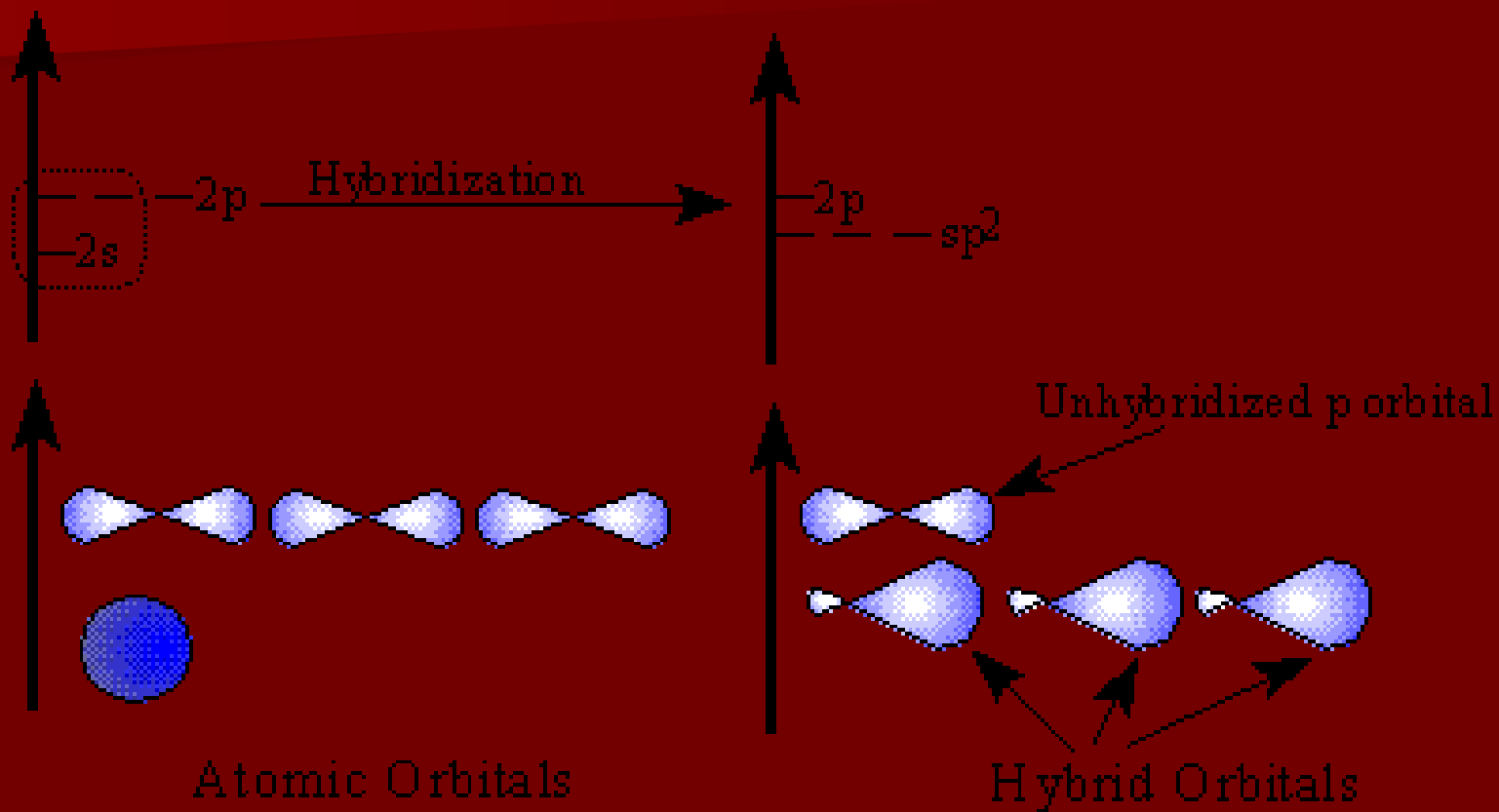


- Based on this hybridization process, the final picture of the molecule is to the left. The Hydrogens have s orbitals represented as the red spheres. They attach to the tips of the hybrid lobes.
- This is because the areas of maximum electron density will always be at the tips of the lobes. When covalent bonds are formed, they will try to utilize the areas of maximum electron density.
- Also notice that the overall geometry of the compound is a tetrahedron with the desired bond angles.
- [Watch animation](#)

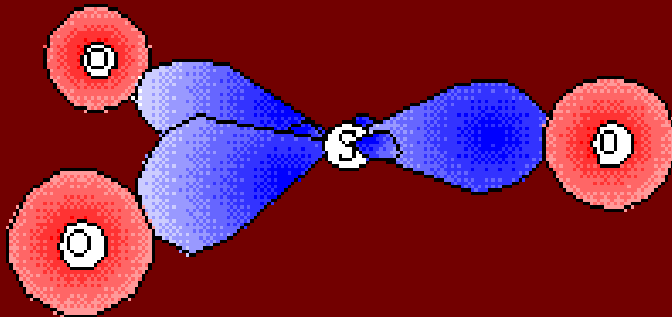
sp^2 hybridized

- Consider Sulfur trioxide- SO_3 -trigonal planar shape-the sulfur must hybridize its atomic orbitals to accommodate the bonding needs of three oxygens with bond angles of 120°
- In order to produce three hybrid orbitals, the Sulfur must hybridize three atomic orbitals.
- Sulfur originally had one s orbital and three p orbitals, it is clear that the one s orbital must be blended with two of the p orbitals
- Note that if the three p orbitals were to be hybridized without the s orbital, then nothing will be accomplished. Identical orbitals will not hybridize to produce anything new





sp^2 hybridized

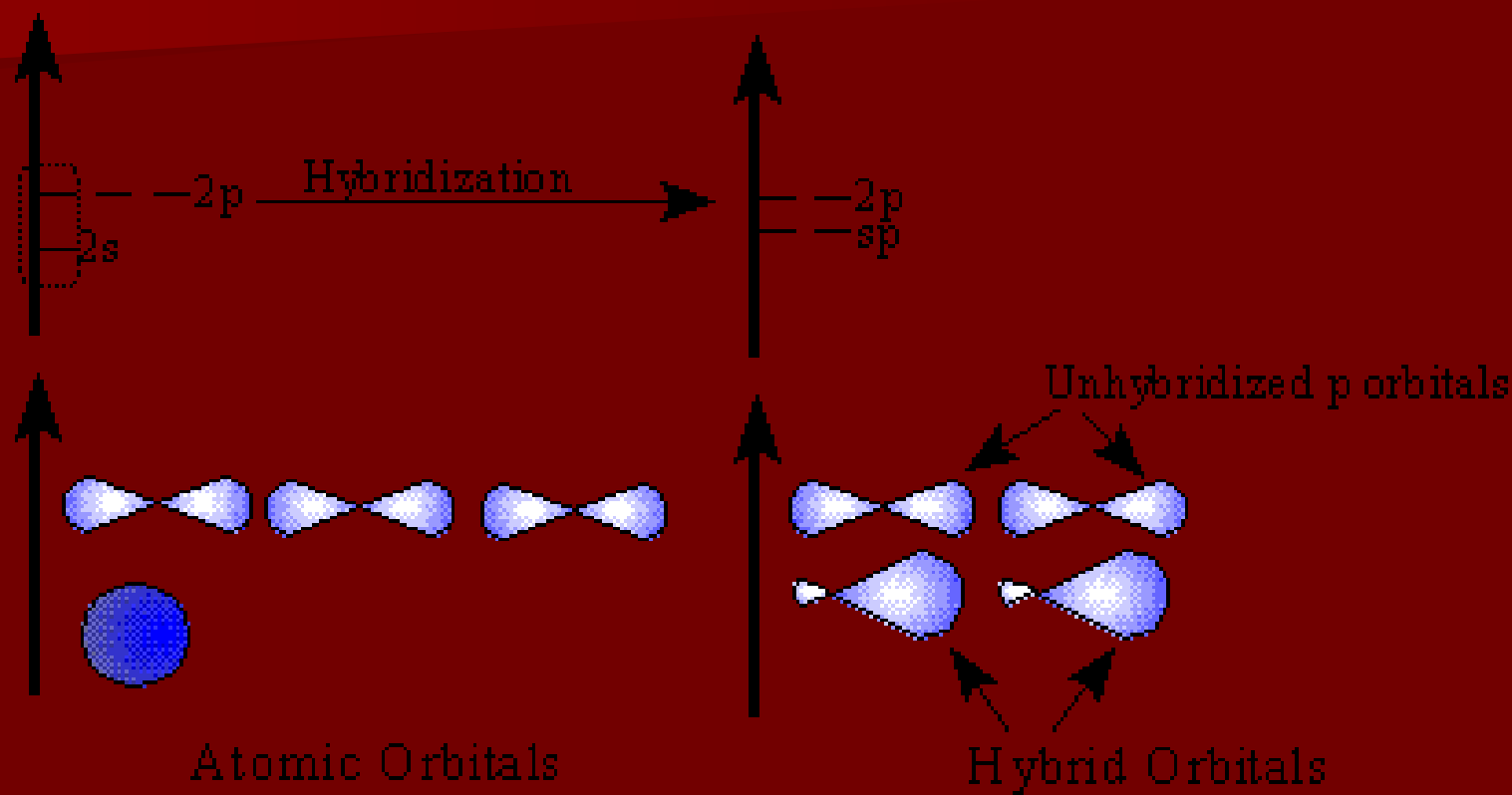


- Based on this hybridization process, the final picture of the molecule is to the left. The oxygen atoms attached to the sulfur at the tips of the hybrid lobes.
- In the picture the three blue orbitals are the Sulfur hybrids. The red spheres are simplified drawings of the three external Oxygen atoms
- Remember there is still one p orbital that wasn't used

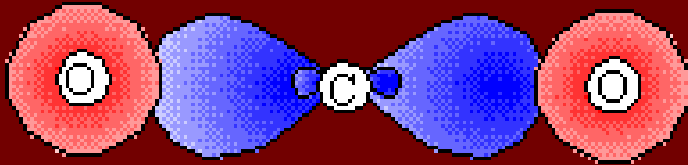
sp hybridized

- Consider Carbon dioxide- CO_2 with 2 electron groups making CO_2 linear with bond angles of 180°
- In the hybridization process, the compound must rearrange itself to attach two atoms to the central Carbon.
- In order to form two hybrids, the system must blend two atomic orbitals.
- In this case, the one s orbital will be combined with one of the p orbitals. Two of the p orbitals will not be involved in the hybridization process.





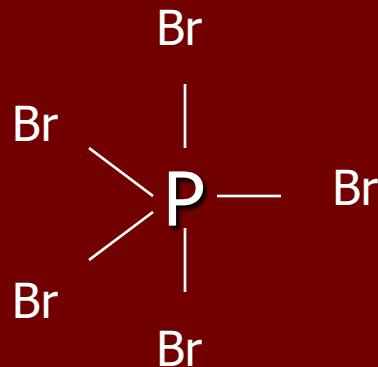
sp hybridized



- Based on the hybridization process the final picture of the molecules is to the left. The compound showing the two attached Oxygen atoms will appear like this. In this diagram the two hybrid orbitals on Carbon are in blue. The Oxygen atoms have been simplified for clarity here and are drawn in red.

dsp^3

- Example PBr_5 electron configuration is:
- $1s^2 2s^2 3s^2 3p^3$
- So the P atoms needs 5 orbitals that are equal, so we get 5 by using dsp^3 hybrid orbitals
- 1 orbitals from s, 3 from p and 1 from d
- The Lewis diagram will look like:

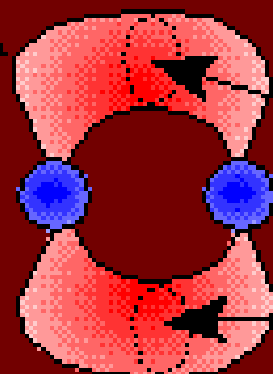
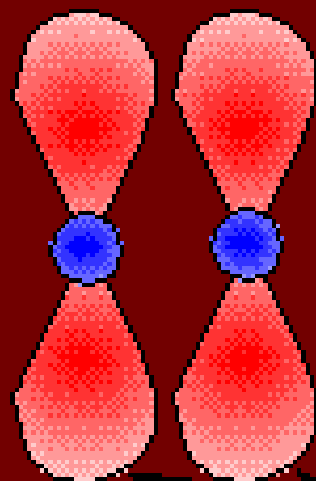


With each Br having a full octet, P has an expanded octet

What happens to the left over p orbitals after hybridization has taken place?

- The left over p orbitals are used to construct the extra bonds between two atoms.
- When multiple bonds appear around an atom, the extra bonds are present to fulfill octet requirements.
- These extra bonds do not need to be as strong as the bonds formed by the hybrids and are always formed from unhybridized p orbitals.
- The extra bonds are formed by aligning two parallel p orbitals on two adjacent atoms.

Bond formed by the overlap of the p orbitals through areas of low electron density



This bond places the maximum electron density at these two locations.

Parallel, unhybridized p orbitals

Sigma and Pi Bonds

- In Hybridization Theory there are two names for bonds: sigma and pi. Sigma bonds are the primary bonds used to covalently attach atoms to each other. Pi bonds are used to provide the extra electrons needed to fulfill octet requirements
- A Sigma bond is a bond formed by the overlap of two hybrid orbitals through areas of maximum electron density. This corresponds to the orbitals combining at the tips of the lobes in the orbitals
- A Pi bond is a bond formed by the overlap of two unhybridized, parallel p orbitals through areas of low electron density. This corresponds to the orbitals combining at the sides of the lobes

Sigma and Pi Bonds

- **The primary bond used to connect two atoms to each other is the sigma bond.**
- **Any additional bonds between two atoms will be pi bonds.**
- **The sigma bond is the stronger of the two types because of its effective use of areas of maximum electron density.**
- **The pi bonds are weaker and more vulnerable to chemical attacks. This is primarily because pi bonds locate maximum electron density between the bonding nuclei but off to the sides a little bit.**
- **A single bond is always a sigma bond.**
- **A double bond is a sigma bond and a pi bond.**
- **A triple bond is a sigma bond and two pi bonds.**

For Practice

- SiF_4
- BCl_3
- CCl_4
- CO_2
- AlI_3

Predict hybridization and show orbitals of them. Give it a try