Hybrid Orbitals
&
Valence Bond Theory

Chapter 11

Hybridization

- Valence *s, p,* and (sometimes) *d* orbitals combine to make ***hybrid orbitals***.
- One hybrid orbital is needed for each electron region – whether it is a single, double, or triple bond.
  - 2 electron regions: sp
  - 3 electron regions: sp^2
  - 4 electron regions: sp^3
  - 5 electron regions: sp^3d
  - 6 electron regions: sp^3d^2

Valence Bond Theory

- **Main Principle:** Atomic orbitals (hybridized or unhybridized) overlap to form covalent bonds between atoms.
- **Orbital overlap** means that the electrons in the bond have a higher probability of being found in the space between the two nuclei.
- **Sigma Bond (σ)** – Bond in which the electron density is greatest along the axis of the bond. The first bond between two atoms is a sigma bond.
- **Pi Bond (π)** – Bond in which the electron density is greatest above and below the axis of the bond. The 2nd and 3rd bonds between two atoms are pi bonds.

sp hybridization

- **BeH_2** is a covalent compound that exists as a LINEAR molecule.
- In the electron dot structure, we see that both of the valence electrons from **Be** form bonds.
- However, in the electron configuration and in the Aufbau diagram for **Be**, we see that both of the valence electrons are already paired:

Be = $1s^22s^2$ **2nd E level**: [↑↓] [ ][ ][ ]
s p p p

sp hybridization

- In order for Be to form two covalent bonds, it must have two unpaired electrons.
- Therefore, one electron must be promoted to the 2p sublevel.

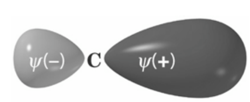
2nd E level: [↑] [↑][ ][ ]
s p p p

- However, an s orbital & p orbital will not allow for the linear shape observed for the **BeH_2** molecule.
- The s & p orbitals then hybridize to create two equivalent sp orbitals that can take on a linear arrangement:

Hybridized 2nd E level: [↑][↑] [ ][ ]
sp sp p p

Hybridization

- When s & p orbitals overlap, they form hybrid orbitals.
- The resulting orbitals have shapes that reflects the shape of both original orbital wave functions.



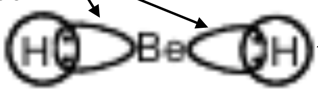
sp hybridization

- The hybridized orbitals of the Be then overlap with the half-filled s-orbital from hydrogen

Be Hybridized 2nd E level: [↑][↑] sp sp   [ ][ ] p p

1s orbital from one H atom → [↓] s   [↓] s ← 1s orbital from a second H atom

Be sp hybrid orbitals



H 1s orbital

sp^2 hybridization

- **BH_3** is a covalent compound that exists as a TRIGONAL PLANAR molecule.
- Boron needs 3 unpaired electrons to make three bonds to hydrogens.
- However, in the electron configuration and in the Aufbau diagram for **Be**, we again see that two of the valence electrons are already paired:

B = $1s^2 2s^2 2p^1$ **2nd E level**: [↑↓] s   [↑][ ][ ] p p p

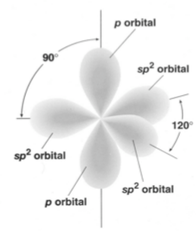
sp^2 hybridization

- One electron will be promoted from the 2s to the 2p sublevel.
- The one 2s orbital and two of the three 2p orbitals will hybridize to make 3 equivalent sp^2 orbitals:

B hybridized 2nd E level: [↑][↑][↑] sp^2 sp^2 sp^2 [ ] p

- The three hybrid orbitals assume a trigonal planar arrangement.
- The hybrid orbitals overlap with the 1s orbitals of 3 hydrogens to create *sigma* bonds.

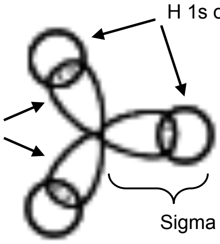
sp^2 hybridization



BH_3 orbital overlap diagram

H 1s orbital

B sp^2 orbitals



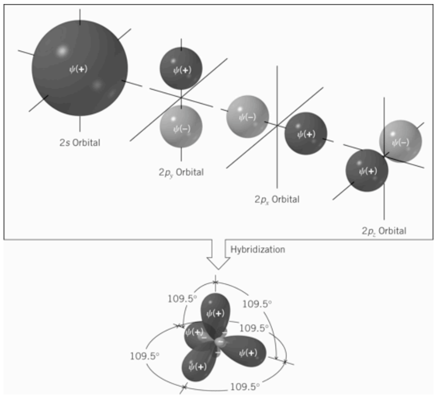
Sigma Bond

sp^3 hybridization in CH_4

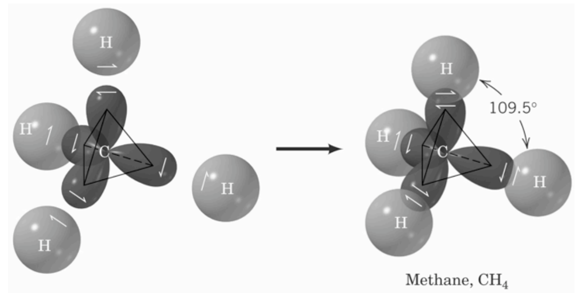
- Methane (CH_4) is a covalent compound that exists as a TETRAHEDRAL molecule.
- Four hybrid orbitals are needed for carbon to make four bonds to hydrogens.
- The one 2s and three 2p orbitals of the 2nd energy level hybridize to make four degenerate (same energy) sp^3 hybrid orbitals.

[↑↓] s   [↑][↑][ ] p p p → [↑][↑][↑][↑] sp^3 sp^3 sp^3 sp^3

Hybridization – sp^3



Bonding in Methane: sp^3 hybridization & orbital overlap



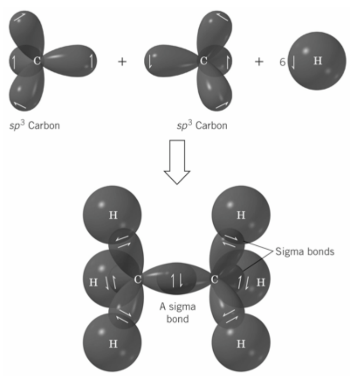
Bonding in Ethane: sp^3 hybridization & VB theory

Consider the electron dot structure of ethene, C_2H_4.

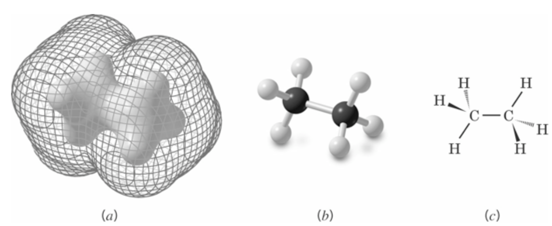
The carbon will require sp^3 hybridization.

Sigma Bond (σ):

Bond in which the electron density is greatest along the axis of the bond. The first bond between two atoms is a sigma bond.

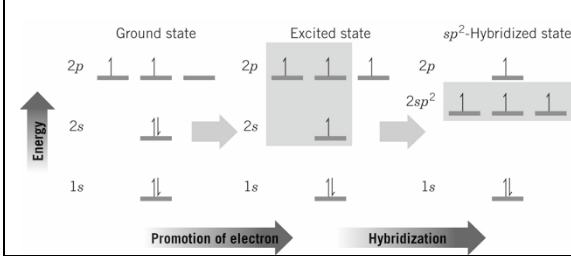


Ethane

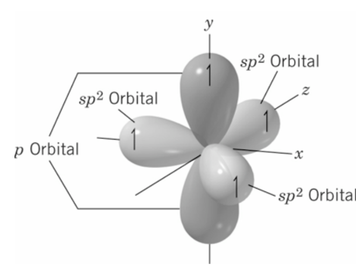


Bonding in Ethene: sp^2 hybridization

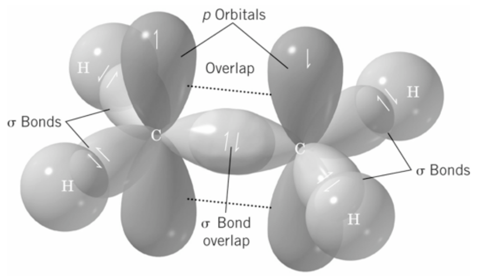
- ***Consider the electron dot structure of ethene, C_2H_4.***
- To form the three bonding regions present around each carbon of ethene, 3 hybrid orbitals are needed – sp^2 hybrid orbitals are formed. A p-orbital is left over.



Bonding in Ethene: sp^2 hybridization



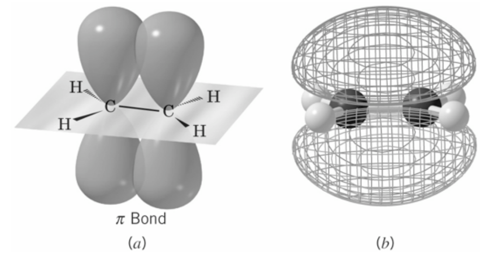
Bonding in Ethene: sp^2 hybridization



Ethene: p-overlap & π bonding

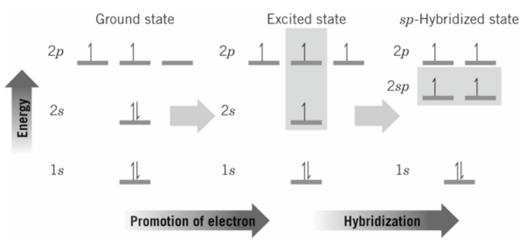
Pi (π) bond:

Bond in which the electron density is above and below the axis connecting two bonded nuclei.

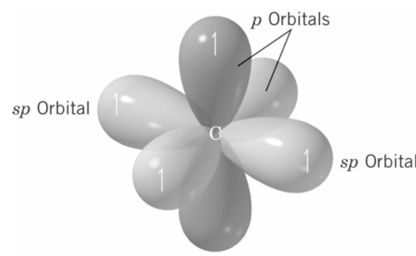


Bonding in Ethyne: sp hybridization

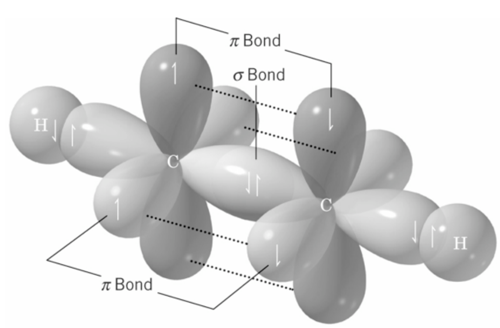
- ***Consider the electron dot structure of ethyne, C_2H_2.***
- To form the two bonding regions present around each carbon of ethyne, 2 hybrid orbitals are needed – sp hybrid orbitals are formed:



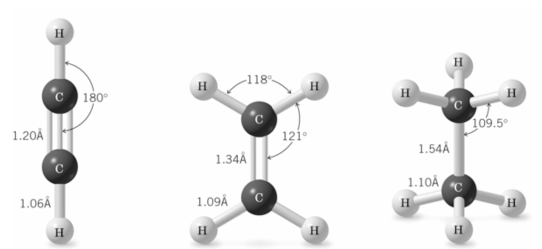
Bonding in Ethyne: sp hybridization



Bonding in Ethyne: sp hybridization



Bond lengths & angles in C_2H_x



1 Å = 1 angstrom = 1 x 10^{-10}