1

Hybridization of Atomic Orbitals

CHAPTER 9

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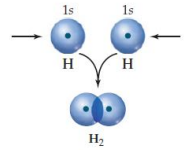
Single bonds

- Bonding electrons are in between atoms
- Bonds form when orbitals overlap



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Potential energy vs distance btw atoms

- When two atoms repel each other, what kind of potential energy is in the system?
- When two atoms attract each other, what kind of potential energy is in the system?
- When bonding, do molecules want to have high or low potential energy?

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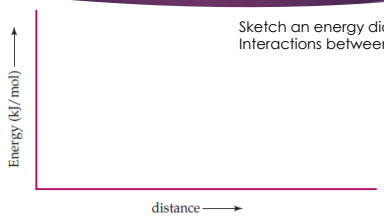
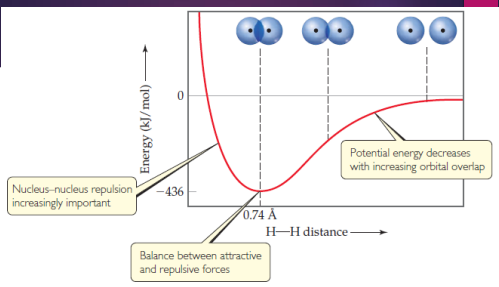
Potential energy vs distance btw atoms

Sketch an energy diagram for Interactions between two atoms





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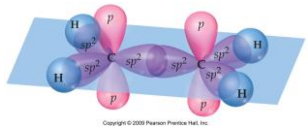
Two Types of Bonds

- Sigma bonds (σ) from overlap of orbitals- **PURPLE**
- Pi bond (π) above and below atoms- **PINK**



Something we have ignored…

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- The Lewis dot diagrams for elements, such as C, N or O do not adequately explain/predict how these atoms actually use their orbitals to form bonds
- A hybridization model was developed in order to explain the bond length/angles and molecular geometry that molecules were experimentally shown to have

Why do we need this hybrid model?

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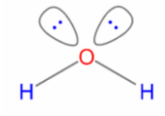
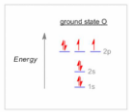
- Consider water:



- Facts: O-H bond lengths are equivalent; lone pairs are equivalent

Orbitals and Electrons in H_2O



- Each H atom has a single electron ($1s^1$)
- The O atom has 8 total electrons ($1s^2 2s^2 2p^4$), with orbitals filled as shown in diagram
- The two lone pairs on O ($2s^2$ and the 2 e^- in the first 2p orbital) are not equivalent (shape, size and energy differences between s and p) so logically they should **not** have the same impact on overall geometry…
  - Experiments show that they actually **are** equivalent
    - Need a new orbital model that reflects this

Hybridization Model for O

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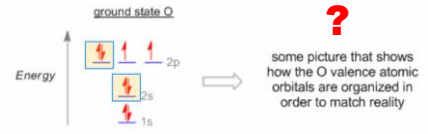
- The lone pairs are not the same here so we need to modify orbital diagram to better match how O bonds in H_2O



Orbital Hybridization

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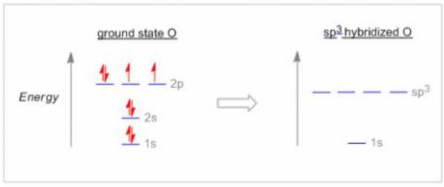

sp^3 Orbital Hybridization

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- Hybridizing (mixing) 1 s orbital and 3 p-orbitals results in 4 sp^3 orbitals
  - All 4 orbitals are equivalent in size, shape and energy
  - Each orbital is ¼ "s-like" and ¾ "p-like" and will look somewhere in between these 2 shapes
  - Notice the number of orbitals hybridized is indicated by the superscript

sp³ Hybridization

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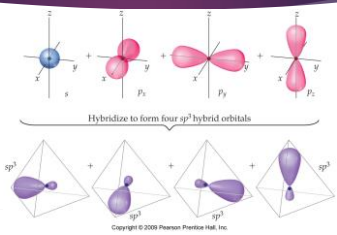

Filling the Hybridized Orbitals

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- The O in H_2O has equivalent lone pairs (sp^3) with this new orbital model
- Two half-filled sp^3 orbitals that will make sigma bonds by overlapping the $1s^1$ orbital

Final shape of H_2O sp^3 Hybrid

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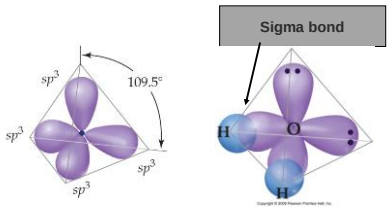

Another Example of sp^3: (CH_4)

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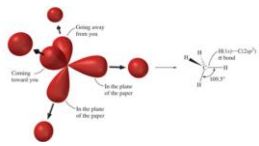
- The four sp^3 orbitals from C project to the four corners of a regular tetrahedral to minimize electron repulsion



sp^3 Orbital Diagrams for C, N and O

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- sp^3 orbitals only form sigma bonds and will not have any pi bonds due to lack of unchanged p-orbitals

Types of Hybrid Orbitals (s and p only)

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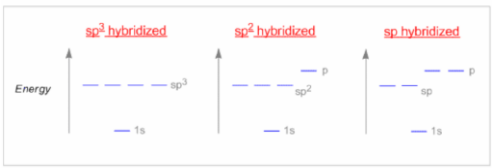

sp² Hybrid Orbitals

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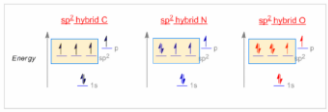
- The sp^2 hybrids are made from 1 s-orbital and 2 p-orbitals, leaving one p orbital unhybridized
- sp^2 orbitals make 3 single (sigma) bonds and the 1 unhybridized p-orbital will make 1 pi bond



sp² Hybridization

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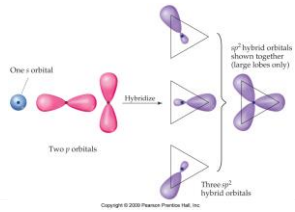

Example of sp² Hybridization

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- Ethylene (ethane) : C_2H_4
  - 3 hybrid sp^2 orbitals = 3 sigma bonds
  - Leaves one p-orbital perpendicular to sigma bond axis which forms a pi bond (double bond)
  - 3 electron domains so VSEPR shape is trigonal planar

Ethylene Molecule (C_2H_4) Where are the sp² hybrid orbitals?

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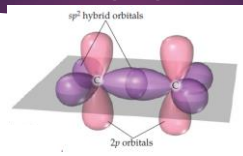

- Hybrid orbitals overlap end-on with s-orbitals of hydrogen atoms; this results in sigma (σ) bond formation
- 1 sigma bond between carbon atoms

Ethylene Molecule (C_2H_4) Where are the p orbitals?

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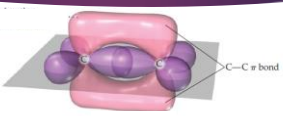

- Orbitals shaded in **pink** are unhybridized p-orbitals that lie at right angles to the plane of the hybrids
- These overlap with each other laterally, which results in the formation of a pi (π) bond.

Ethylene Molecule (C_2H_4) Bonding

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- C=C consists of 1 σ bond and 1 π bond
- C—H consists of 1 σ bond

sp Hybrid Orbitals

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- sp hybrids combine 1 s-orbital and 1 p-orbital, leaving 2 unhybridized p-orbitals

sp Hybridization

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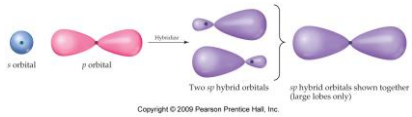
- One s-orbital and one p-orbital combine



sp Hybridization

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- sp hybrids will have 2 electron domains (1 single bond and 1 triple bond)
- 2 domains are located 180° apart to minimize repulsion
- Linear VSEPR shape

sp Hybridization Example

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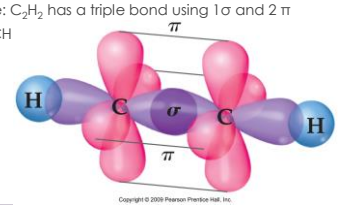
- Ethyne: C_2H_2 has a triple bond using 1σ and 2 π

HC≡CH



C_2H_2

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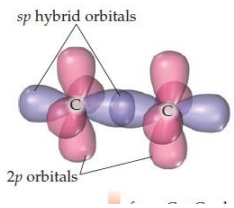
- Start with bond



C_2H_2

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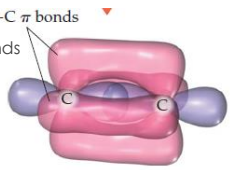
- Overlap π bonds
- C≡C is 1 σ and 2 π bonds



C_2H_2

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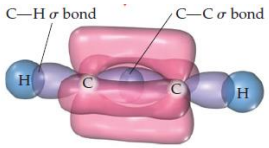
- Add σ bonds for H



Example #1

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Which atom and hybridization pattern does this picture represent?

- A) sp^3 O
- B) sp^2 N
- C) sp N
- D) sp^3 C
- E) sp C

Example #2

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Which atom and hybridization pattern does this picture represent?

- A) sp^3 N
- B) sp^2 O
- C) sp C
- D) sp^2 N
- E) sp^3 C

Example #3

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Which atom and hybridization pattern does this picture represent?

- A) sp C
- B) sp^2 N
- C) sp^3 C
- D) sp^3 O
- E) sp^3 N

Example #4

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Indicate the sp hybrid atom(s) in HCN

Example #5

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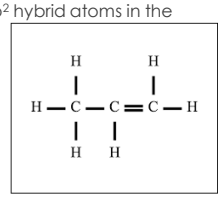
- Label the sp^3 and sp^2 hybrid atoms in the following molecule



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Example #6

- If the bond angle in SeH_2 is measured to be 90˚, what does this tell you about the hybridization of Se?