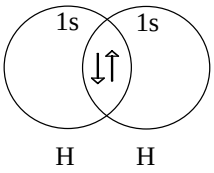
5.111 Lecture Summary #15

Readings for today: Sections 3.4, 3.5, 3.6 and 3.7 (Sections 3.4, 3.5, 3.6, 3.7, and 3.8 in *3rd ed*) – Valence Bond Theory.
Read for Lecture #16: Sections 6.13, 6.15, 6.16, 6.17, 6.18, and 6.20 (Sections 6.14, 6.16, 6.17, 6.18, 6.19, and 6.21 in *3rd ed*) – The Enthalpy of Chemical Change.

Assignment: Problem set #5 (due Friday, October 17th at noon)

Topics: **Valence bond theory and hybridization**
- **I.** Sigma and pi bonds
- **II.** Hybridization of atomic orbitals
  - **A.** sp^3 hybridization
  - **B.** sp^2 hybridization
  - **C.** sp hybridization

VALENCE BOND THEORY AND HYBRIDIZATION



In **valence bond theory**, bonds result from the pairing of unpaired electrons in atomic orbitals.

I. SIGMA AND PI BONDS

σ (sigma) bond: cylindrically symmetric with ____ nodal plane across the bond axis.

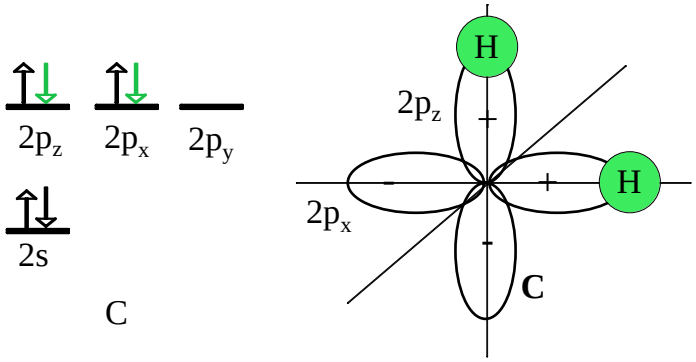
π (pi) bond: a bond with e^- density in two lobes, one on each side of the bond axis.

A pi bond has a _____ nodal plane along the bond axis.

We can describe multiple bonds according to valence-bond theory.

- single bond: _____
- double bond: one **σ-**bond plus one _____
- triple bond: one **σ-**bond plus _____ π-bonds

Applying simple VB theory results in the following prediction for methane bonding:

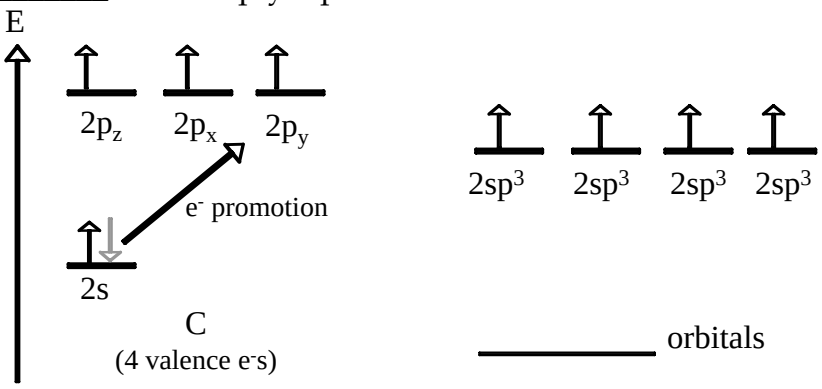


According to this model, the C is bonded to only two H-atoms with an H-C-H bond of _____°. This is NOT what is observed for methane!

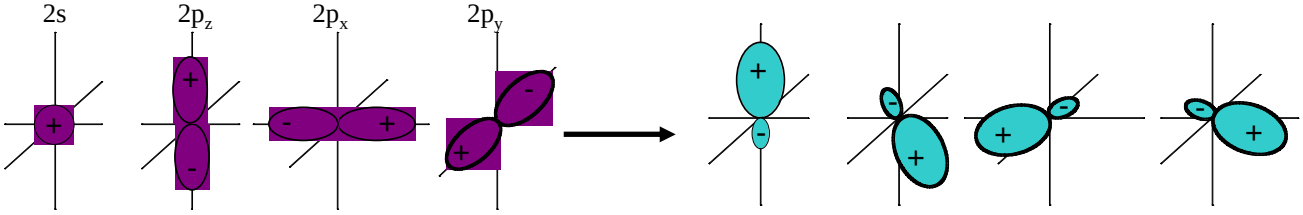
II. HYBRIDIZATION OF ATOMIC ORBITALS

A. sp^3 hybridization

A carbon atom has four unpaired electrons available for bonding once a 2s-electron is _____ to an empty 2-p orbital.

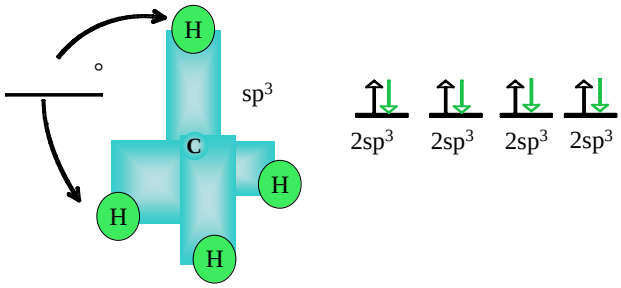


The sp^3 hybrid orbitals are equivalent and degenerate. They differ only in their _____ in space.



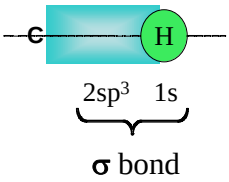
four sp^3 hybrid orbitals

In carbon, each sp^3 orbital contains a single electron, allowing four bonds.



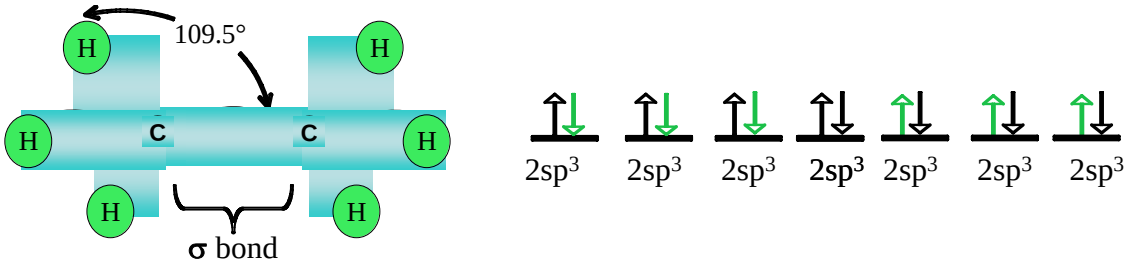
What provides the energy for the initial electron promotion?

_____!



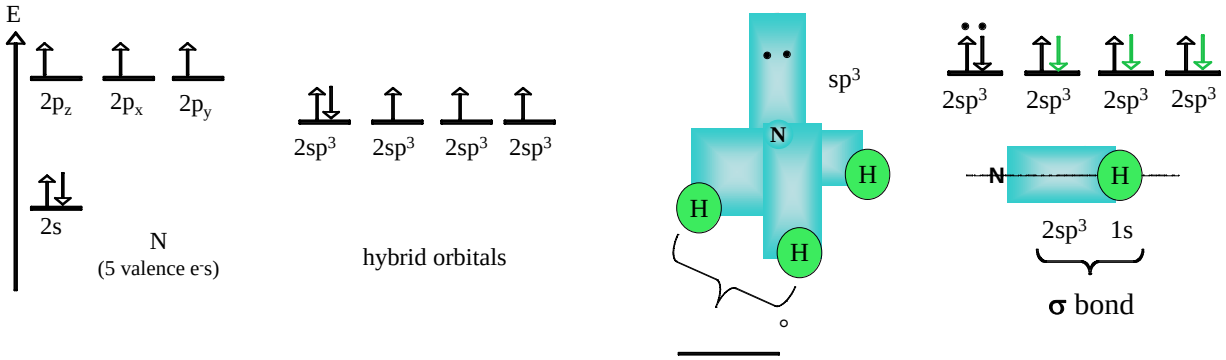
Each bond is labeled based on the bond type (σ or π) and atomic orbital composition. ____ (C_____, H_____)

Consider ethane, C_2H_6.



Two bond types in ethane: _____ and _____ .

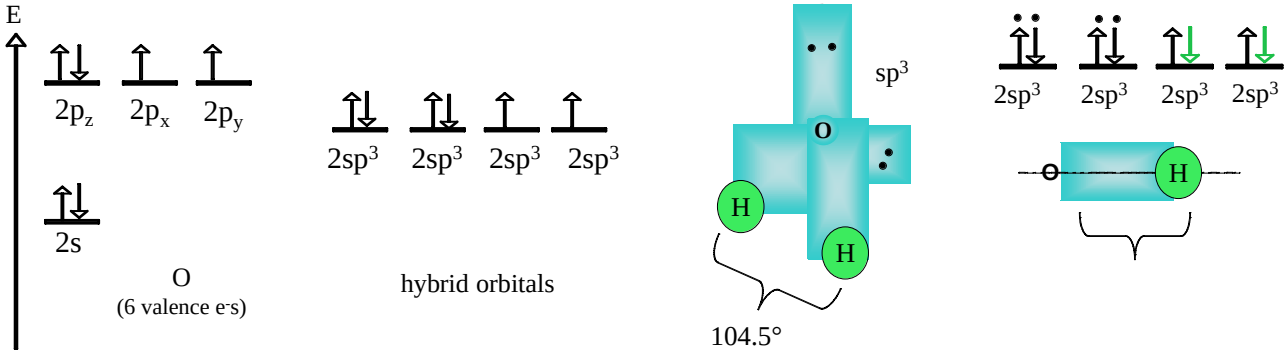
Nitrogen: Electron promotion _____ occur with nitrogen because promotion would not increase the number of unpaired electrons available for bonding.



N-H bond description: _____

N-atom geometry: _____

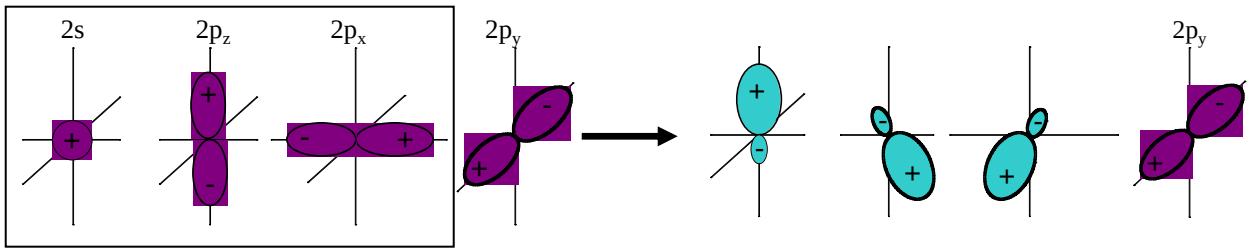
Oxygen: Electron promotion does not occur.



H_2O geometry: _____

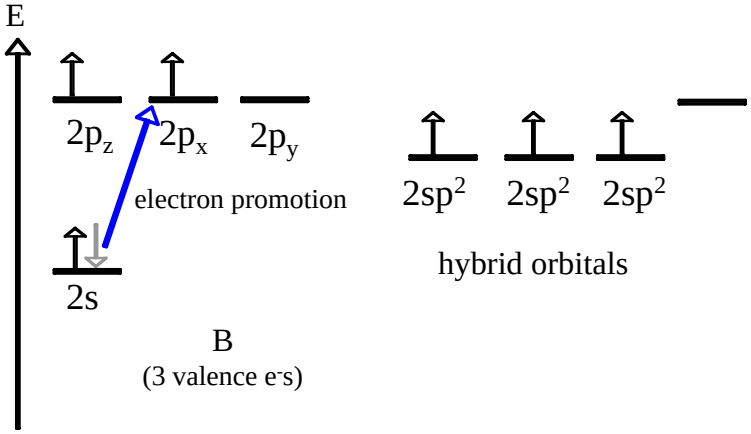
B. sp^2 hybridization

sp^2 hybrid orbitals form from the combination of one s-orbital and two p-orbitals.



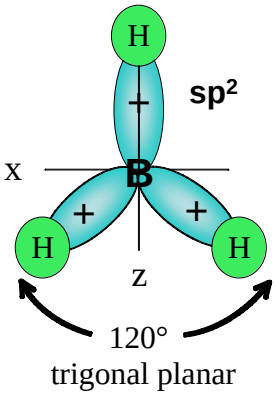
3 hybrid orbitals 1 p-orbital

Boron: Boron has 3 unpaired electrons available for bonding once a 2s-electron is promoted to an empty 2-p orbital.

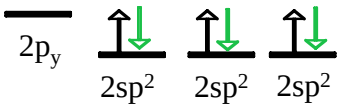


The s-orbital and two of the p-orbitals hybridize to form _____ sp^2 orbitals.

The three sp^2-orbitals lie in a _____ to minimize electron repulsion.

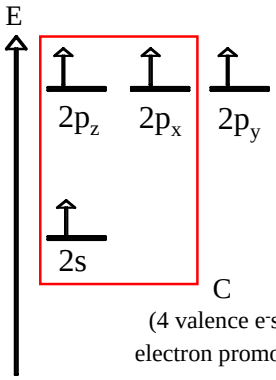


trigonal planar

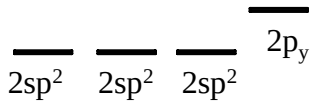


σ (, H1s)

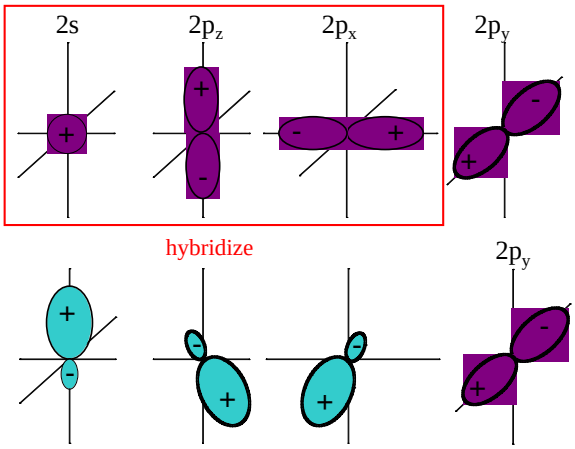
Carbon: Carbon can also form sp^2 hybrid orbitals.

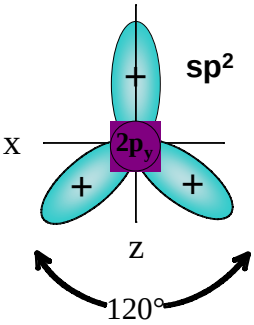


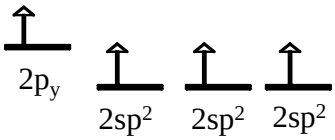
C
(4 valence e⁻s)
electron promotion



hybrid orbitals

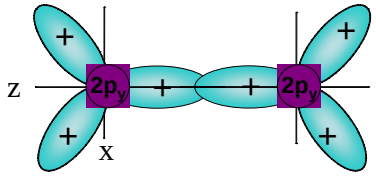






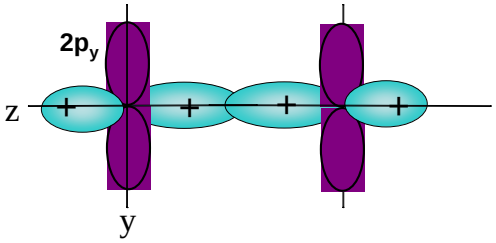
trigonal planar

Ethylene (C_2H_4) has a C-C double bond, meaning one _____-bond and 1 _____-bond.



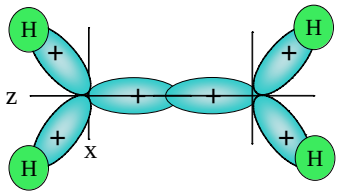
looking down the y-axis

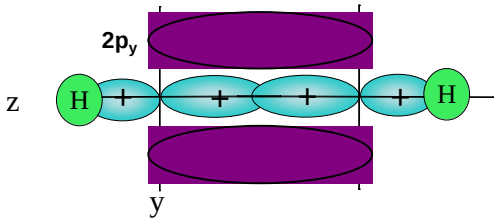
σ(_____, _____)



looking down the x-axis

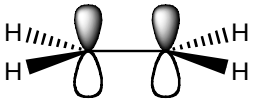
π(_____, _____)



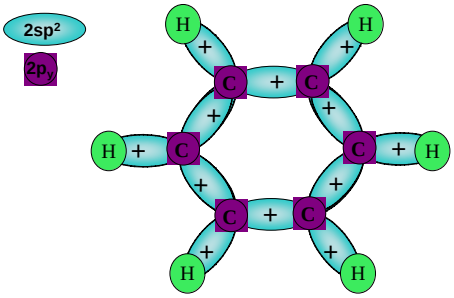


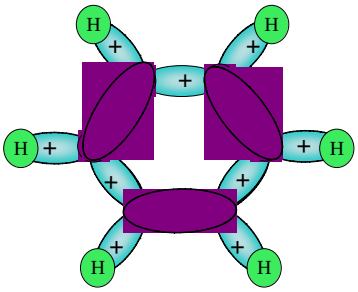
In addition to the C-C double bond, there are four C-H bonds: σ(_____, _____)

Note: molecules cannot rotate around a double bond. Rotation would require breaking the pi bond.



Benzene (C_6H_6)

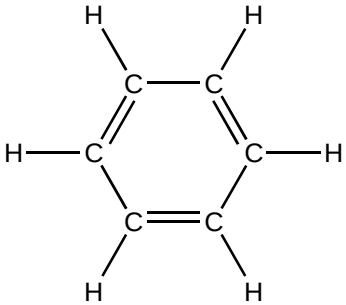


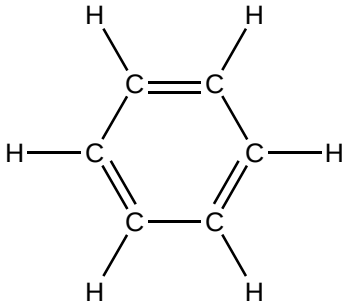


_____ σ(C2sp^2, C2sp^2) bonds

_____ π(C2p$_y$, C2p$_y$) bonds

_____ σ(C2sp^2, H1s) bonds

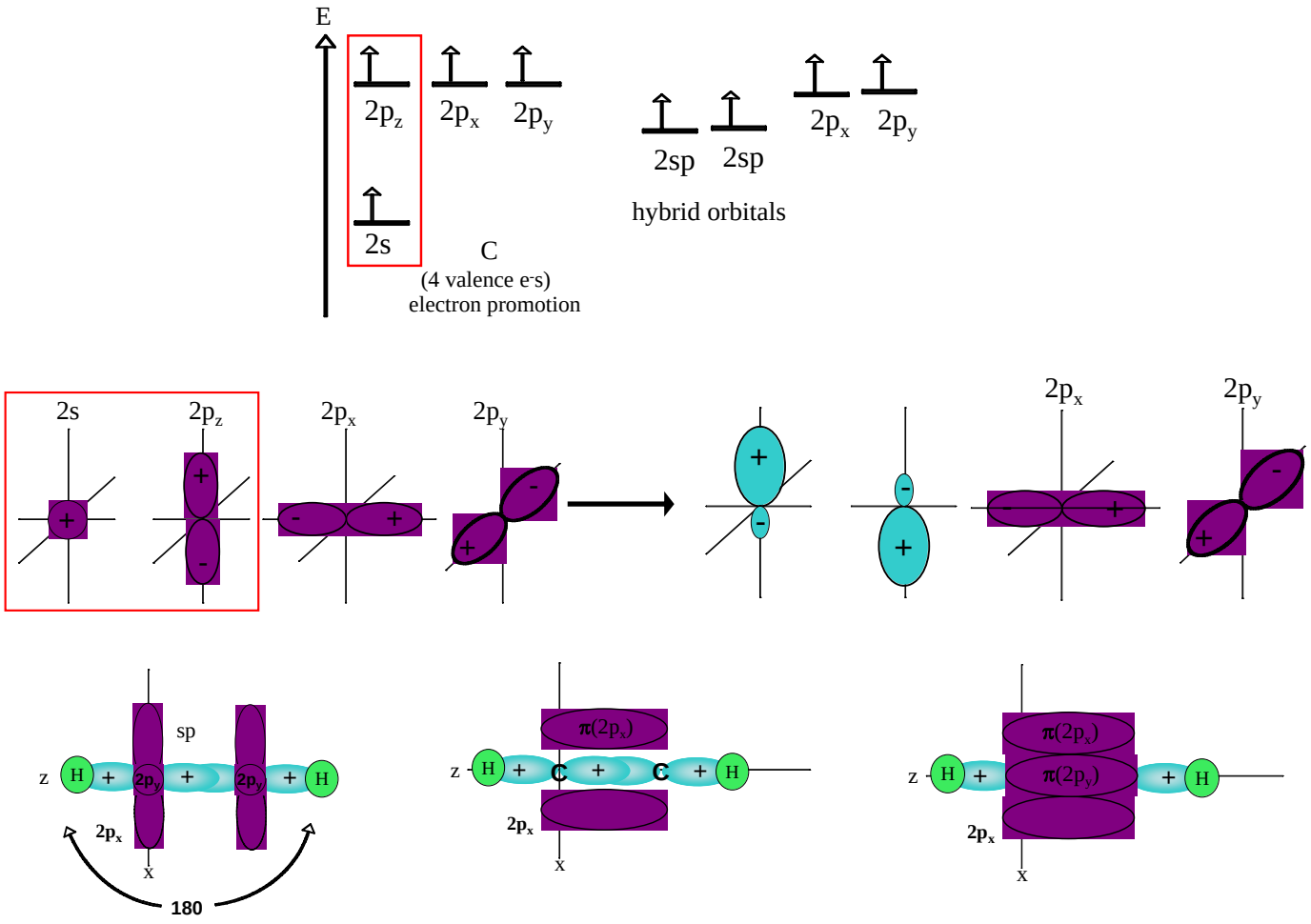




In reality, the 6 pi-electrons are _____ over all six carbon atoms in the benzene molecule. Each C-C bond is a _____ bond.

C. sp hybridization

sp hybrid orbitals form from the combination of one s-orbital and 1 p-orbital.



σ(_____, _____) π(_____, _____) π(_____, _____)

5.111 Principles of Chemical Science

Fall 2008