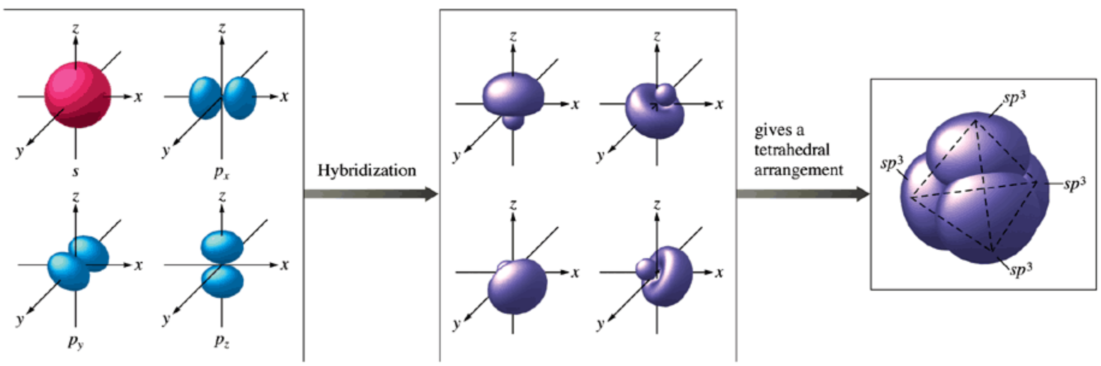
Name _________________________ **AP CHEM** **__/__/__**

Chapter 9 Outline – Covalent Bonding: Orbitals

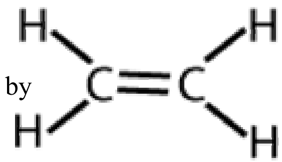
Hybridization and the Localized Electron Model

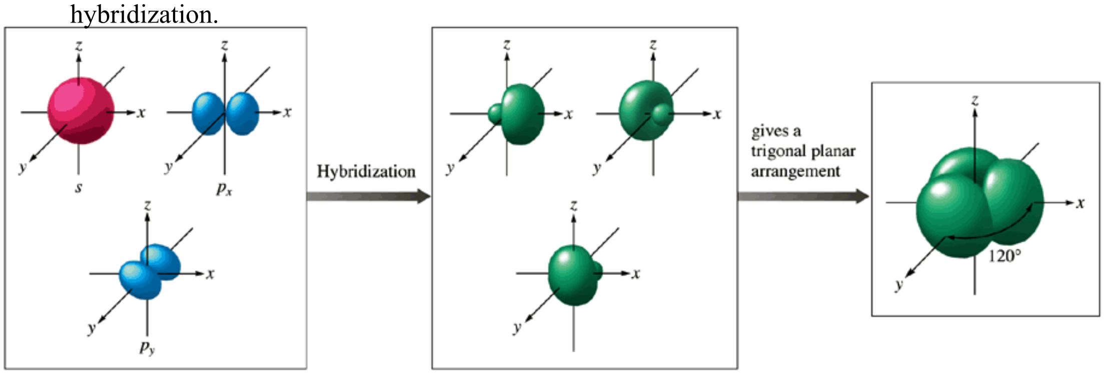
- **sp^3 Hybridization**
  - In general we assume that bonding only involves valence electrons.
  - Consider methane (CH_4).
    - The valence electrons of hydrogen use 1s orbitals.
    - The 2p and 2s atomic orbitals of carbon will lead to two different type of C—H bonds: those from the overlap of the carbon 2p orbital with the 1s orbital of hydrogen and those from the overlap of a carbon 2s orbital with the 1s orbital of hydrogen.
    - This is not the case. The methane molecule is tetrahedral with bond angles of 109.5° So either the localized electron model is wrong or carbon adopts a set of orbitals other than its "native" 2s and 2p orbitals to bond to the hydrogen atoms in forming the methane molecule.
    - The 2s and 2p orbitals present on an isolated carbon atom may not be the best set of orbitals for bonding. It makes sense to assume that the carbon atom has four equivalent atomic orbitals arranged tetrahedrally.
    - Such a set of orbitals can be obtained by combining the carbon 2s and 2p orbitals as shown below.

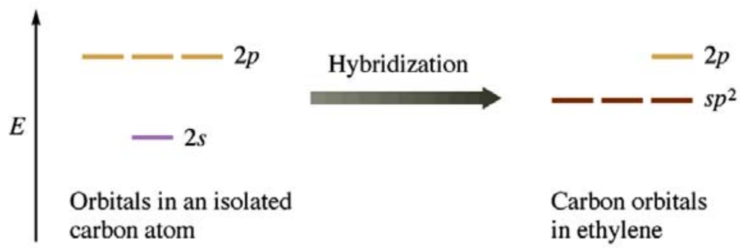


    - This mixing of the native atomic orbitals to form special orbitals for bonding is called hybridization.
    - The four new orbitals are called sp^3 orbitals because they are formed from one 2s orbital and three 2p orbitals(s^1p^3).
    - We say that the carbon atom undergoes sp^3 hybridization or is sp^3 hybridized.
    - Whenever a set of equivalent tetrahedral atomic orbitals is required by an atom, this model assumes that the atom adopts a set of sp^3 orbitals; the atom becomes sp^3 hybridized.
    - What the atoms in a molecule were like before the molecule was formed is not as important as how the electrons are best arranged in the molecule. This model assumes that the individual atoms respond as needed to achieve the minimum energy for the molecule.

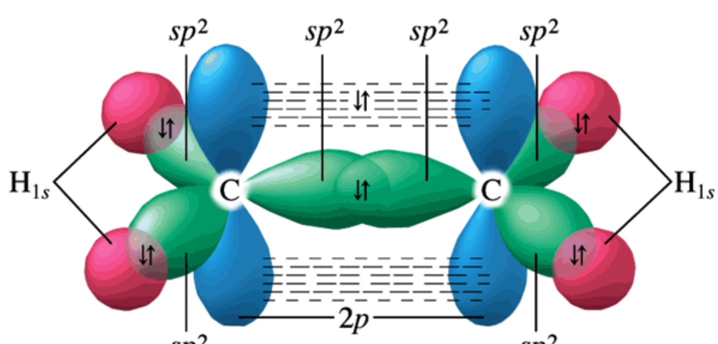
- **sp^2 hybridization**
  - Ethylene (C_2H_4) is an important material in the manufacture of plastics.
  - A double bond acts as one effective pair, so the ethylene is surrounded by three effective pair.
  - This requires a trigonal planar arrangement with bond angles of 120°.
  - Since one 2s and two 2p orbitals are used to form these hybrid orbitals, this is called sp^2 hybridization.





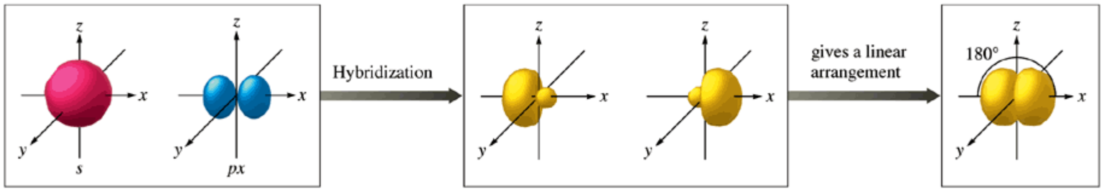


  - In forming the sp^2 orbitals, one 2p orbital on carbon has not been used. This remaining p orbital (p_z) is oriented perpendicular to the plane of the sp^2 orbitals.
  - The three sp^2 orbitals on each carbon can be used to share electrons, as shown below.

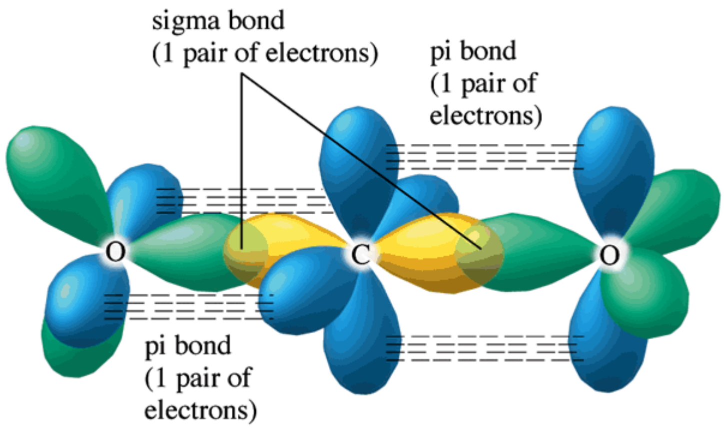


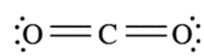
  - In each of these bonds, the electron pair is shared in an area centered on a line running between the atoms. This type of covalent bond is called a sigma(σ) bond. In the ethylene molecule, the σ bonds are formed using sp^2 orbitals on each carbon atom and the 1s orbital on each hydrogen atom.
  - The second bond must therefore result from sharing an electron pair in the space above and below the σ bond.
  - The parallel p orbitals can share an electron pair, to form a pi(π) bond.
  - σ bonds are formed from orbitals whose lobes point toward each other, but π bonds result from parallel orbitals. A double bond always consists of one σ bond where the electrons are located between the atoms and one π bond which occupies the space above and below the σ bond.

- **sp hybridization**
  - In the CO_2 molecule the carbon has two effective pair that will be arranged at an angle of 180°.
  - To obtain two hybrid orbitals arranged at 180° requires sp hybridization, involving one s orbital and one p orbital.



  - Two effective pairs around an atom will always require sp hybridization of that atom.
  - In CO_2 the sp orbitals on carbon form σ bonds with the sp^2 orbitals on the two oxygen atoms. The remaining sp^2 orbitals on the oxygen atoms hold lone pair. The π bonds between the carbon atom and each oxygen atom are formed by the overlap of parallel 2p orbitals.



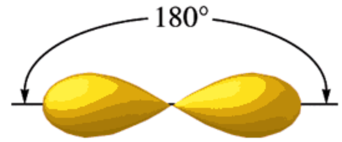
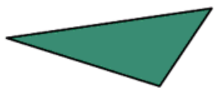
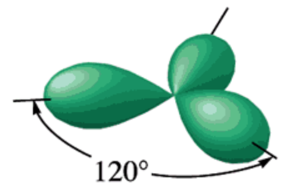
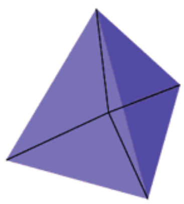
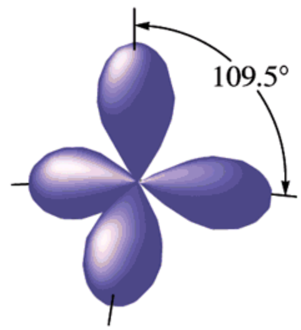
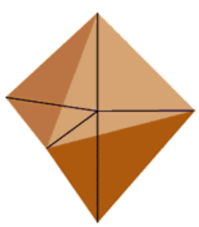
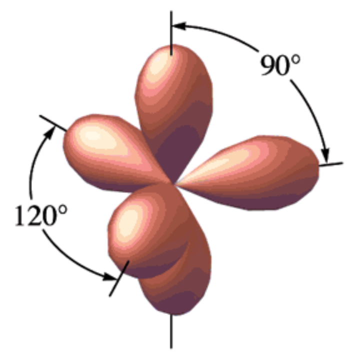


- **dsp^3 hybridization**
  - Since 5 pairs of electrons are needed for atoms such as phosphorus in PCl_5, a dsp^3 hybridization is necessary.
  - The dsp^3 hybridized phosphorus atom in PCl_5 molecule uses its 5 dsp^3 orbitals to share electrons with five chlorine atoms.
  - A set of five effective pairs around a given atom always requires a trigonal bipyramidal arrangement which in turn requires dsp^3 hybridization of that atom.

- **d^2sp^3 hybridization**
  - Since 6 pairs of electrons are needed for atoms such as sulfur in SF_6, a d^2sp^3 hybridization is necessary.
  - A set of six effective pairs around a given atom always requires an octahedral arrangement which in turn requires d^2sp^3 hybridization of that atom.

Paramagnetism

- Most materials have no magnetism until they are placed in a magnetic field. However, in the presence of such a field, magnetism of two types can be induced.
- Paramagnetism causes a substance to be attracted to the inducing magnetic field.
- Diamagnetism causes the substance to be repelled from inducing magnetic field.
- Studies have shown that paramagnetism is associated with unpaired electrons and diamagnetism is associated with paired electrons.
- The O_2 molecule is known to be paramagnetic.

Number of Effective Pairs	Arrangement of Pairs		Hybridization Required	
2		Linear	*sp*	
3		Trigonal planar	sp^2	
4		Tetrahedral	sp^3	
5		Trigonal bipyramidal	dsp^3	
6		Octahedral	d^2sp^3