10/4/11 VSEPR

hybridization

structural molecular orbital graphs

common organic molecules

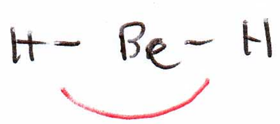
VSEPR - valence shell electron pair repulsion

The valence shell contains the most energetic electrons → the ones that participate in bonding

- Electrons tend to occur in either lone or bonding pairs
- Like charges (such as electrons) repel

- The shapes of molecules are generated by valence electrons trying to get as far away from each other as possible,

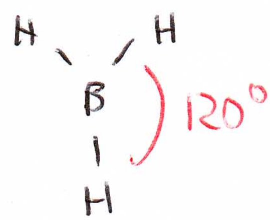
Prototype shapes - shapes due only to bonds



180°

linear

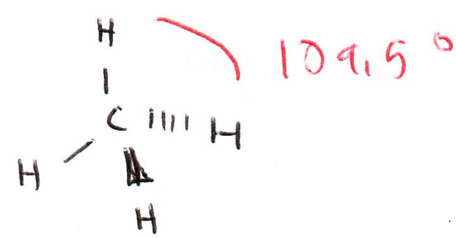
sp



borane

trigonal planar

sp^2



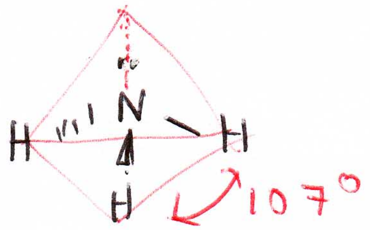
methane

tetrahedral

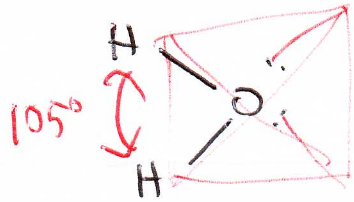
sp^3

When a lone pair is present, it causes distortion of the molecular geometry due to the fact that lone pairs have more effective repulsive force than bonding pairs of electrons.

Derivative shapes - shapes due to the distortion of lone pairs



ammonia
trigonal pyramidal
sp^3



bent
sp^3

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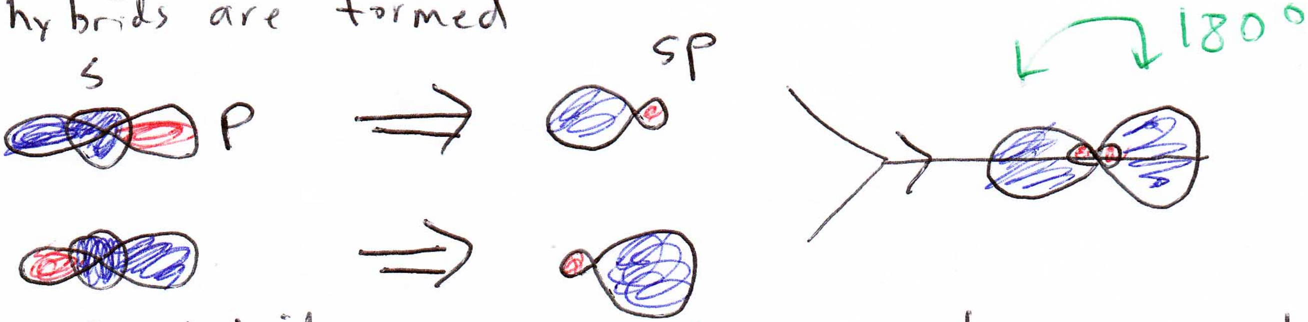
hybridization

- AOs cannot be used directly to describe molecules since molecules have multiple nuclei; the shapes of AOs are due to there being exactly and only one nucleus present.
- hybrids are formed by adding + subtracting orbitals from the <u>same</u> atom (LCAO) to create a new set of molecular orbitals that are equal in energy and match the geometry of the system.
- hybridization is determined by geometry → # of hybrids needed = # of lone pairs + σ bonds

How hybrids are formed



# of hybrids generated is always equal to the # of AOs used.

Structural Molecular Orbital Graphs → SMOGs

These diagrams show the kind of orbitals present (not phase) to demonstrate the structure of a molecule.

convention: simplified hybrids : 

$CH_4 \rightarrow 4\ \sigma\ \text{bonds} \rightarrow 4\ \text{hybrids} \rightarrow 4\ \text{AOs} \rightarrow s,p,p,p \rightarrow sp^3$

s

sp^3

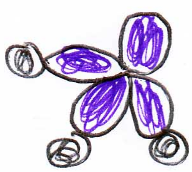
before: $\frac{\uparrow\downarrow}{2s}$ $\underbrace{\frac{\uparrow}{}\ \frac{\uparrow}{}\ \frac{}{}}_{2p}$ | after: $\underbrace{\frac{\uparrow}{}\ \frac{\uparrow}{}\ \frac{\uparrow}{}\ \frac{\uparrow}{}}_{sp^3}$

CH_3^- – methyl anion

carbanion – an anion (–) on carbon

H–C(H)(H): ⊖

3 σ bonds + lone pair → 4 hybrids → 4 AOs → s,p,p,p → sp^3



CH_3^+ – methyl cation

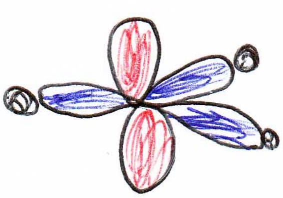
carbocation – a cation (+) on carbon

H–C⊕(H)–H

only 3 σ bonds → 3 hybrids → s,p,p → sp^2

before: $\frac{\uparrow\downarrow}{2s}$ $\underbrace{\frac{\uparrow}{}\ \frac{}{}\ \frac{}{}}_{2p}$ | $\underbrace{\frac{\uparrow}{}\ \frac{\uparrow}{}\ \frac{\uparrow}{}}_{sp^2}$ $\frac{}{p}$

leftover p orbital!



s

sp^2

p

Since individual electrons do not have the repulsive force of pairs of electrons, single electrons do not affect geometry, so they do not affect hybridization.

$CH_3\cdot$ — methyl radical