10/3/11

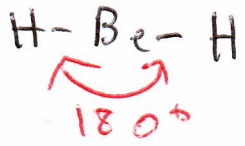
VSEPR
hybridization
Structural Molecular Orbital Graph
common organic molecules

VSEPR- valence shell electron pair repulsion

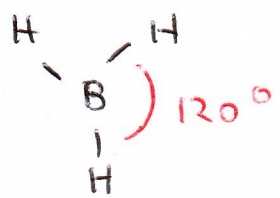
→ The valence shell contains the most energetic electrons — the ones that participate in bonding

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

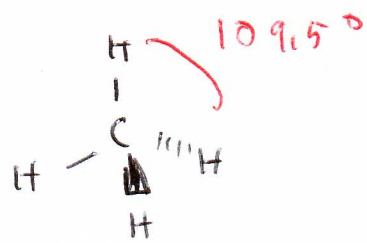
-The shapes of molecules are generated by electrons trying to get as far away from each other as possible.



linear
sp



borane
trigonal planar
sp^2

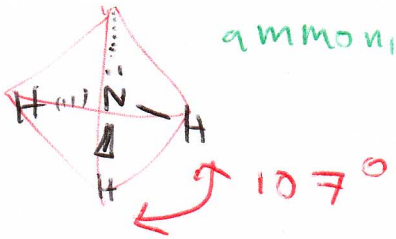


methane
tetrahedral
sp^3

Prototype shapes

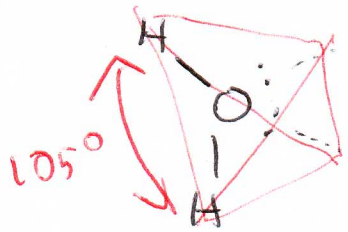
These three shapes are formed in cases where there are no lone pairs. When lone pairs are present, they will distort the geometry slightly since lone pairs have slightly more repulsive force than bonds.

ammonia



trigonal Pyramidal

sp^3



bent

sp^3

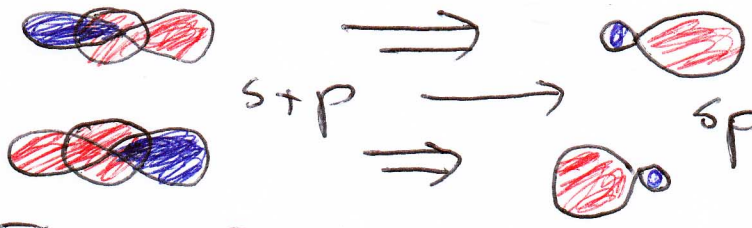
Derivative shapes - shapes formed due to the distortion of lone pairs.

Hybridization

- LCAO — atomic orbitals from the same atom are added + subtracted in such a way as to create a new set of orbitals that are equal in energy and match the geometry of the system.
- AOs cannot be directly used to describe molecules since molecules have multiple nuclei, and the AOs are formed by the presence of one nucleus.

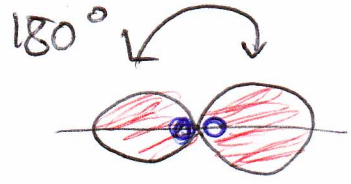
* Hybridization is determed by geometry → determined by # of lone pairs and σ bonds

How hybrids are formed



written

simultaneously

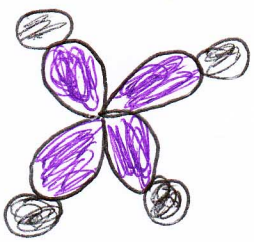


The # of hybrids generated is always equal to the # of AOs used.

Structural Molecular Orbital Graphs → SMOGs

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

CH_4 → 4 bonds → 4 hybrids → s, p, p, p → sp^3



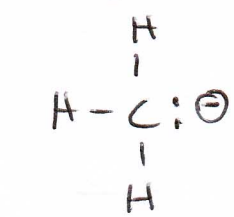
s
sp^3

simplified hybrids

For clarity, only the major lobe of hybrids is being shown.

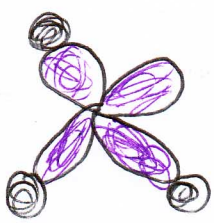
C: $\underset{2s}{\uparrow\downarrow}$ $\underset{2p}{\uparrow}$ $\underset{}{\uparrow}$ $\underset{}{-}$ ⟹ $\underset{sp^3}{\uparrow}$ $\uparrow$ $\uparrow$ $\uparrow$

CH_3^-



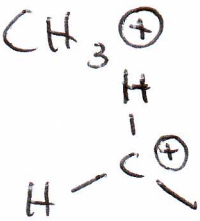
4 hybrids are still needed → 4 AOs → sp^3

carbanion → an anion (− charge) on carbon



trigonal pyramidal

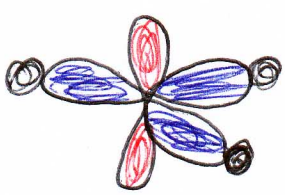
CH_3^+



carbocation → a cation (+ charge) on carbon

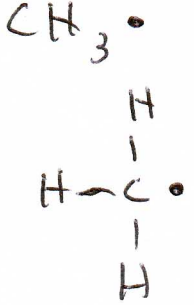
only 3 hybrids are needed because there are only 3 bonds → sp^2

C: $\underset{2s}{\uparrow\downarrow}$ $\underset{2p}{\uparrow}$ $\underset{}{\uparrow}$ $\underset{}{-}$ ⟹ (mixing 1 e⁻) $\underset{sp^2}{\uparrow}$ $\uparrow$ $\uparrow$ $\underset{2p}{-}$



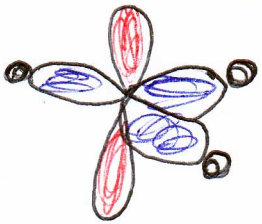
s
sp^2
p

#4



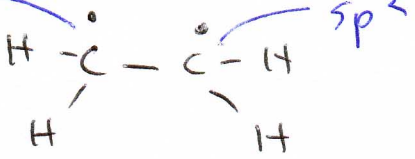
radical – a molecule with an unpaired e^-

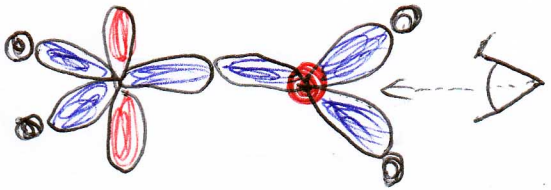
– lone electrons do not have the repulsive force of lone or bonding pairs of electrons. ~~The~~ Therefore, single electrons do not affect geometry, so they do not affect hybridization.

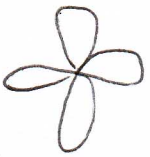


end of quiz #1

$\dot{C}H_2 - \dot{C}H_2$ sp^2







p orbitals must be @ 90° to each other.