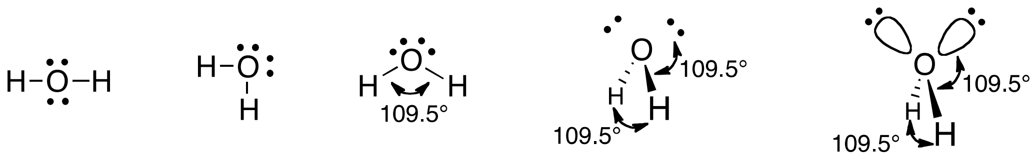
# SD Shape of Molecules: VSEPR

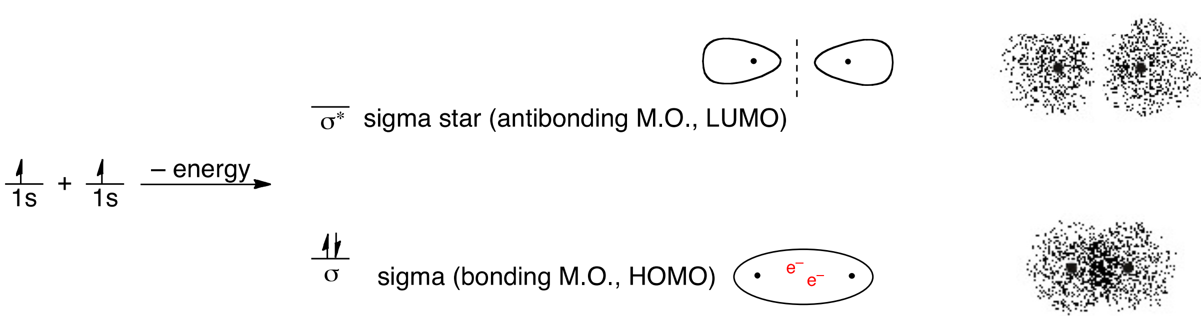
Valence Shell Electron Pair Repulsion




Handout page 1

# 3D Shape of Molecules: Molecular Orbital (MO) Theory

- M.O.'s are described by mathematical equations
- Aufbau Principle: Fill lowest energy orbital first
- Pauli exclusion principle: pair spins of electrons
- Hund's Rule: Fill degenerate orbitals
- Start with Atomic Orbitals (A.O.'s) (or hybridized A.O.'s)
- Overlap end-to-end or 1s-to-end gives a sigma (σ) bond
- Overlap of unhybridized p orbitals gives a pi (π) bond

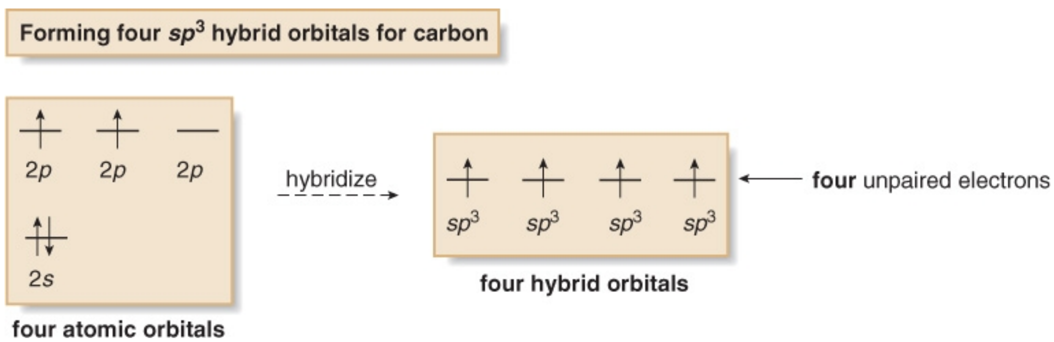



The Orbital dot diagrams are from: http://www.meta-synthesis.com/webbook/39_diatomics/diatomics.html

# Orbitals and Bonding: Methane

Chemists have proposed that atoms like carbon do not use pure *s* and pure *p* orbitals in forming bonds. Instead, atoms use a set of new orbitals called hybrid orbitals.

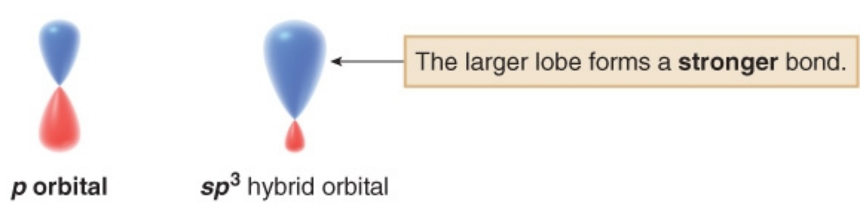
*Hybridization* is the combination of two or more atomic orbitals to form the same number of hybrid orbitals, each having the same shape and energy.



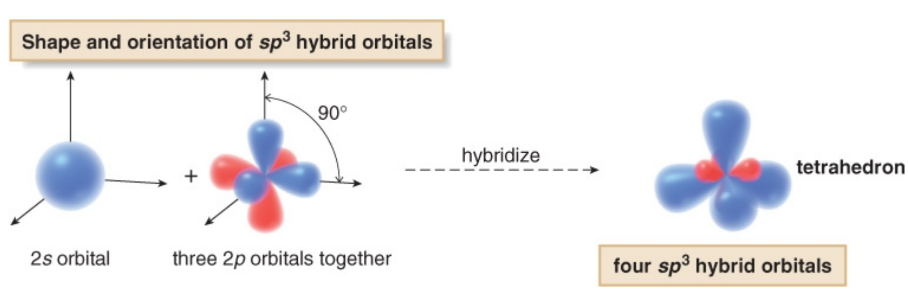



# Shape and Orientation of $sp^3$ Hybrid Orbitals

The mixing of a spherical 2*s* orbital and three dumbbell shaped 2*p* orbitals together produces four hybrid orbitals, each having one large lobe and one small lobe (Figure 1.8).

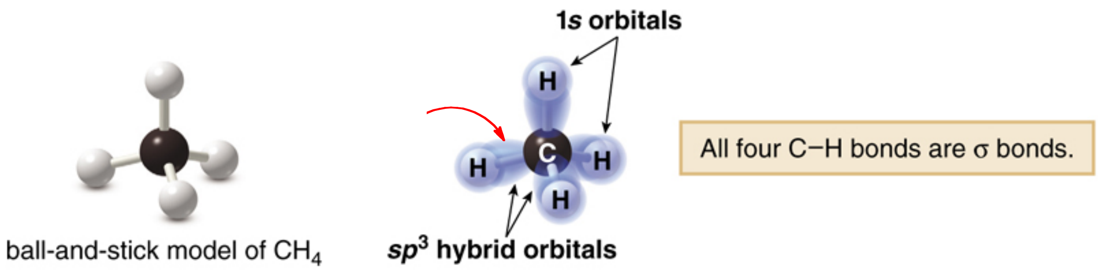



The four hybrid orbitals are oriented towards the corners of a tetrahedron, and form four equivalent bonds.



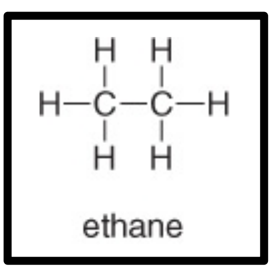
# Bonding Using *sp*³ Hybrid Orbitals

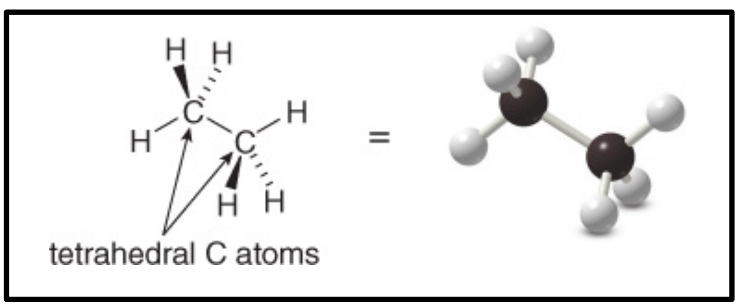
Each bond a sigma bond (σ) in $CH_4$ is formed by overlap of an $sp^3$ hybrid orbital of carbon with a 1*s* orbital of hydrogen. These four bonds point to the corners of a tetrahedron.

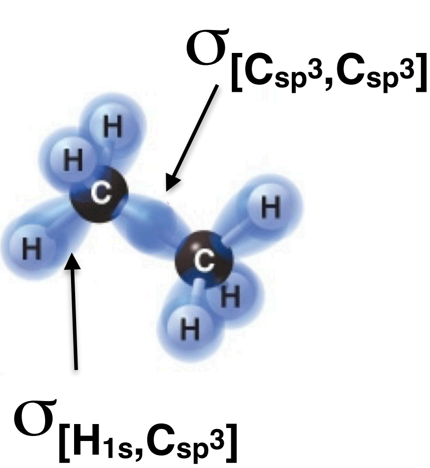


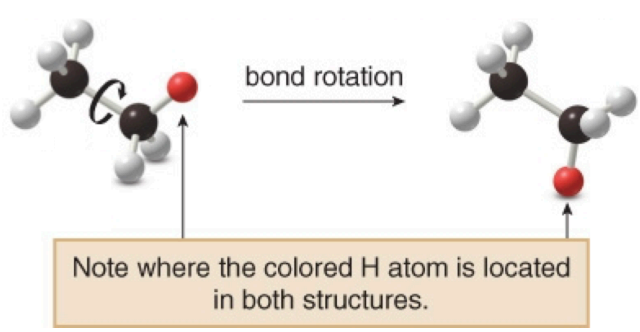



# Hybridization and Bonding in Organic Molecules

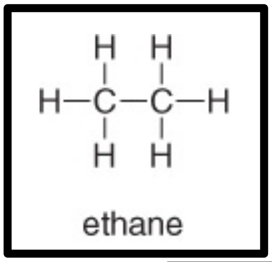


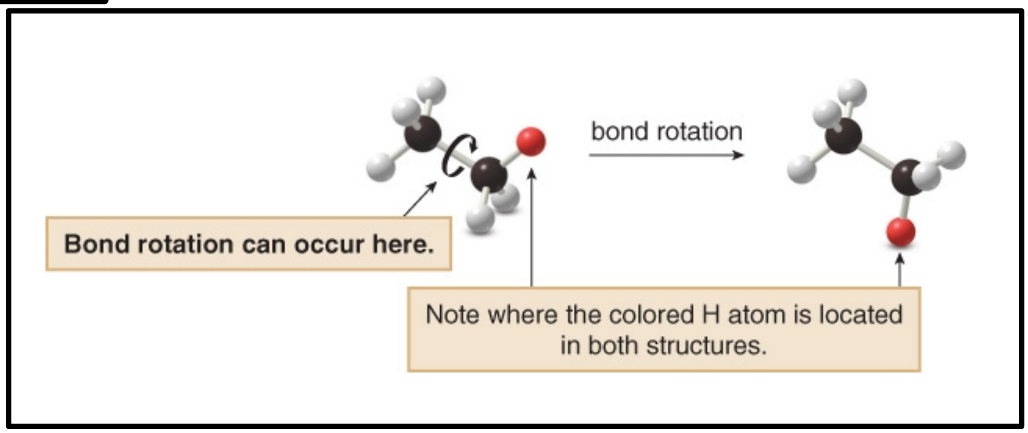



# Hybridization and Bonding in Organic Molecules

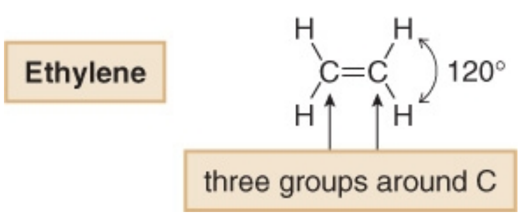



Making a model of ethane illustrates one additional feature about its structure. Rotation occurs around the central C—C σ bond.



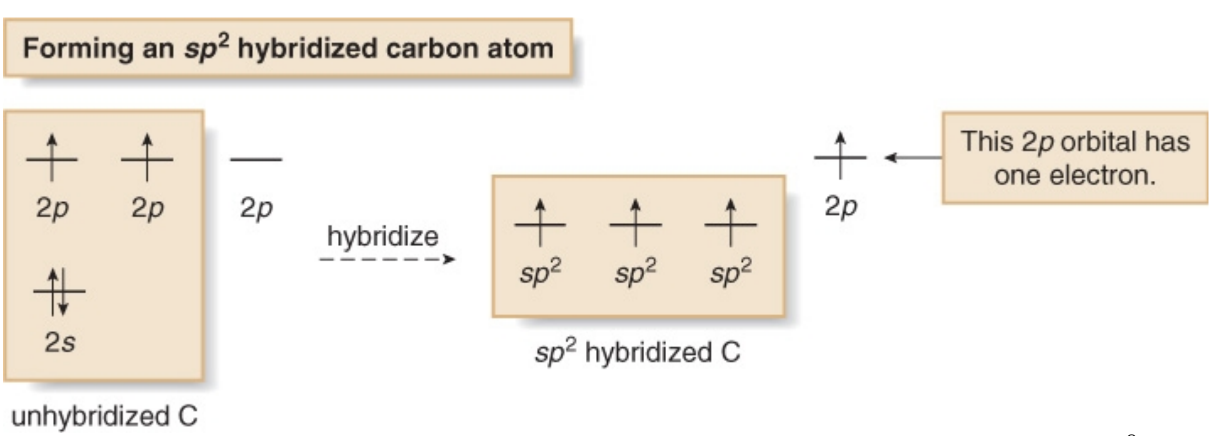



# Hybridization and Bonding in Double Bonded Molecules

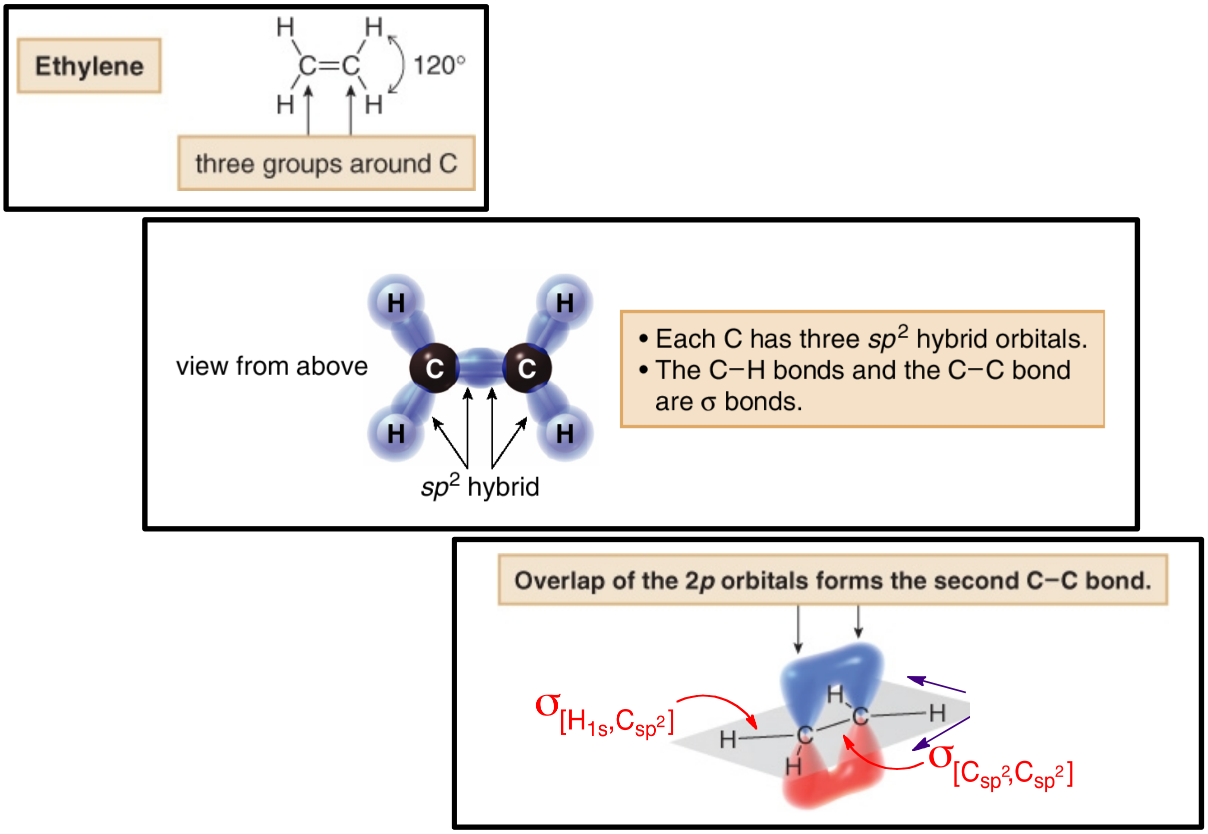



Each carbon is trigonal and planar.

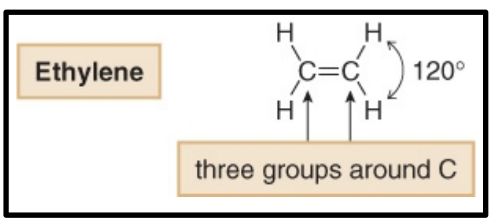
Each carbon is $sp^2$ hybridized



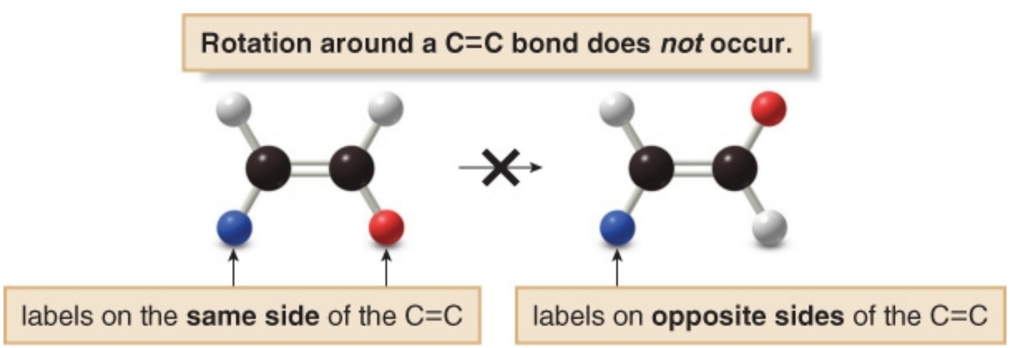
# Hybridization and Bonding in Organic Molecules



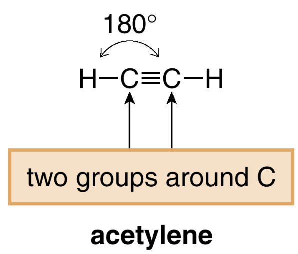

# Hybridization and Bonding in Organic Molecules

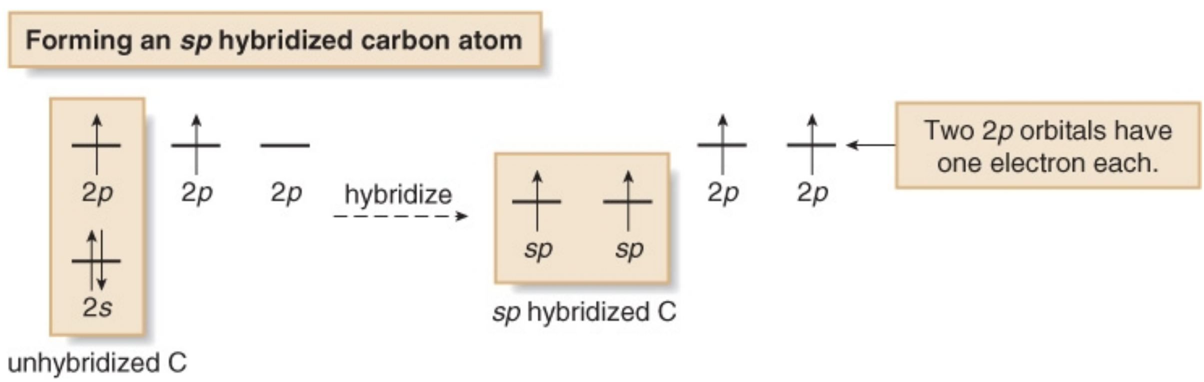



Unlike the C—C bond in ethane, rotation about the C—C double bond in ethylene is restricted. It can only occur if the π bond first breaks and then reforms, a process that requires considerable energy.



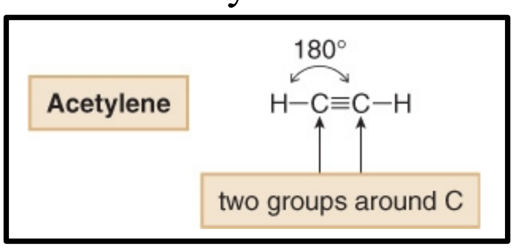
# Hybridization and Bonding in Organic Molecules

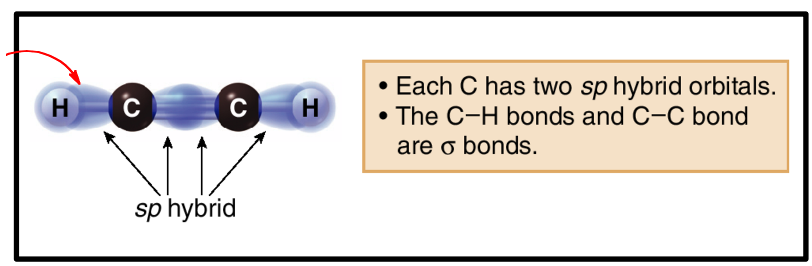


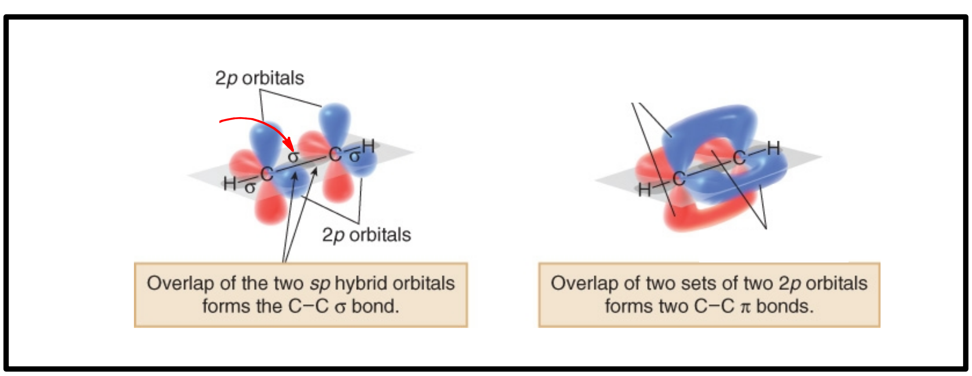






# Hybridization and Bonding in Organic Molecules

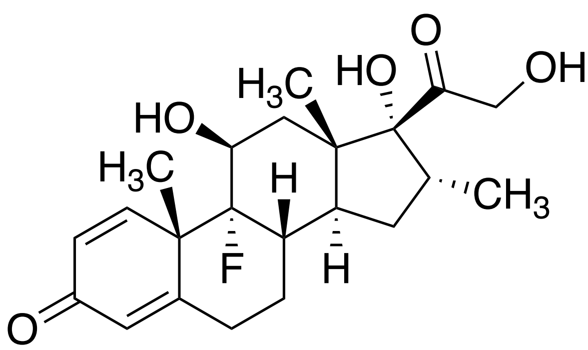


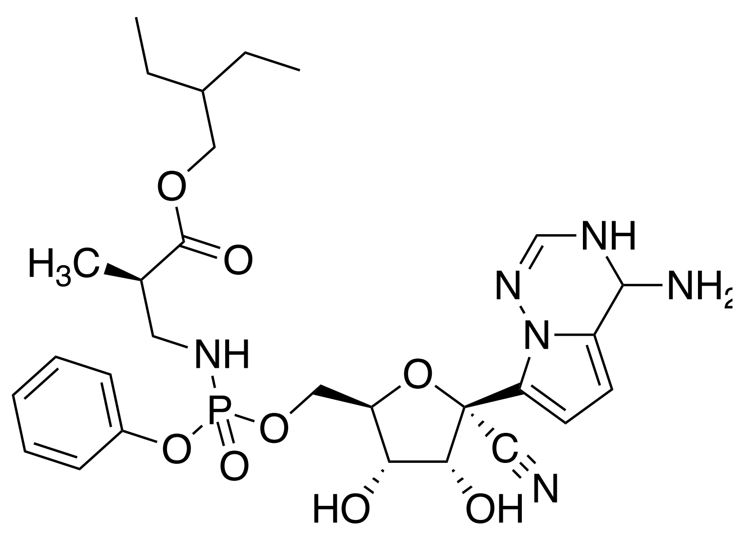



## Hand Draw 3D Model of $CH_3CN$





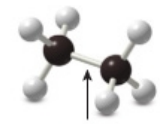
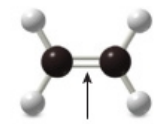
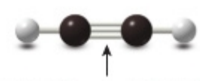

Dexamethasone




Remdesivir

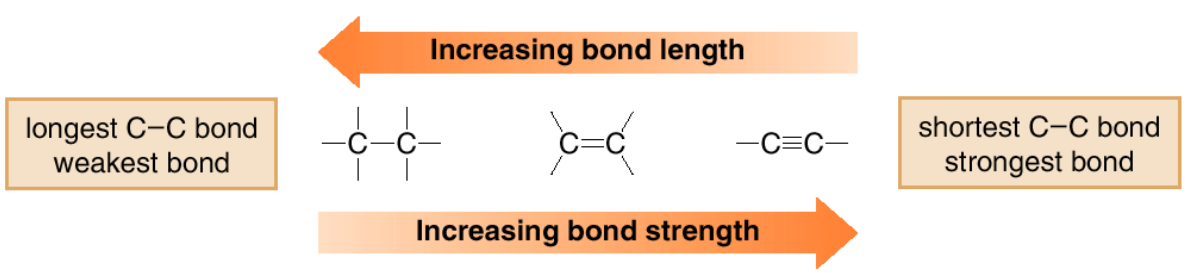
# Summary of Covalent Bonding Organic Compounds

Important Slide: Copy this one down

| Number of groups bonded to C | Hybridization | Bond angle | Example | Observed bonding |
|---|---|---|---|---|
| 4 | $sp^3$ | 109.5° tetrahedral | $CH_3CH_3$ ethane |  one σ bond; $C_{sp^3}–C_{sp^3}$ |
| | | | $CH_2=CH_2$ ethylene |  one σ bond + one π bond; $C_{sp^2}–C_{sp^2}$ + $C_{2p}–C_{2p}$ |
| | | | HC≡CH acetylene |  one σ bond + two π bonds; $C_{sp}–C_{sp}$ + $C_{2p}–C_{2p}$, $C_{2p}–C_{2p}$ |

Note: groups include pairs of nonbonding electrons

# Bond Length and Bond Strength




# **Know trends not numbers**

# Structure and Bonding: Summary



**Table 1.3** Bond Lengths and Bond Strengths for Ethane, Ethylene, and Acetylene

| Compound | C–C bond length (Å) | |
|---|---|---|
| $CH_3-CH_3$ | 1.53 | ↑ Increasing bond length |
| $CH_2=CH_2$ | 1.34 | |
| $HC\equiv CH$ | 1.21 | |

| Compound | C–H bond length (Å) | |
|---|---|---|
| $CH_3CH_2-H$ | 1.11 | ↑ Increasing bond length |
| $CH_2=C(H)-H$ | 1.10 | |
| $HC\equiv C-H$ | 1.09 | |

**Beware: stronger bonds ≠ less reactive**

# Bond Length and Bond Strength

**Increased percent *s*-character - - → Increased bond strength - - → Decreased bond length**

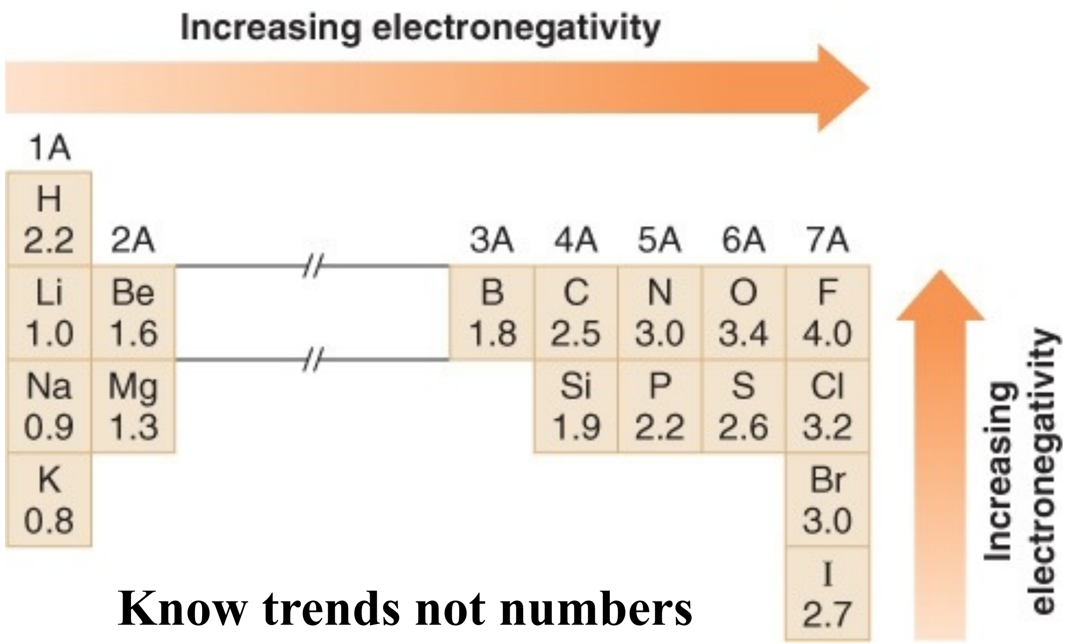
***sp* hybrid** $\frac{\text{one } 2s \text{ orbital}}{\text{two hybrid orbitals}}$ = 50% *s*-character

***sp*² hybrid** $\frac{\text{one } 2s \text{ orbital}}{\text{three hybrid orbitals}}$ = 33% *s*-character

***sp*³ hybrid** $\frac{\text{one } 2s \text{ orbital}}{\text{four hybrid orbitals}}$ = 25% *s*-character

# Electronegativity of the Elements

Electronegativity is a measure of an atom’s attraction for electrons in a bond.



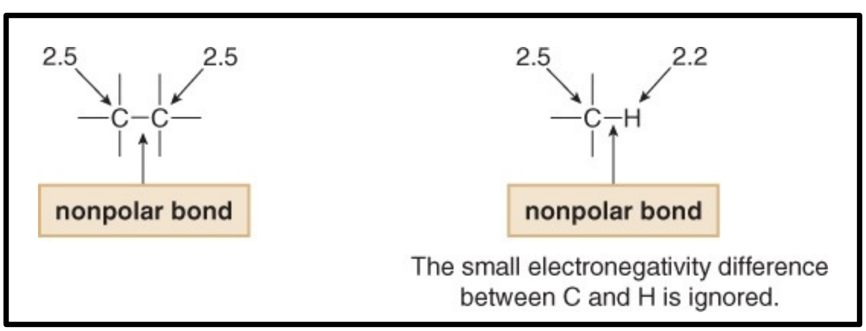

**Know trends not numbers**

19

# Nonpolar vs Polar Bonds

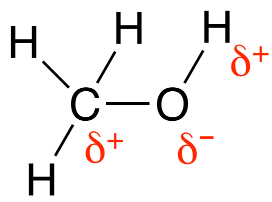
When electrons in a bond are:

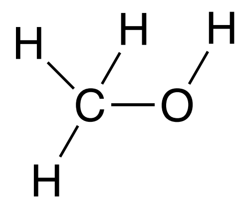
- equally shared, the bond is nonpolar.
- unequally shared, the bond is polar (i.e. a “separation of charge” or a “dipole”)




- C–C bonds are nonpolar.
- C–H bonds are considered to be nonpolar

## Notation of Bond Polarity

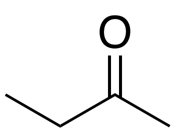


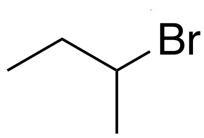




$\delta^+$ means the indicated atom is electron deficient.

$\delta^-$ means the indicated atom is electron rich.

Or use special arrow ( ).



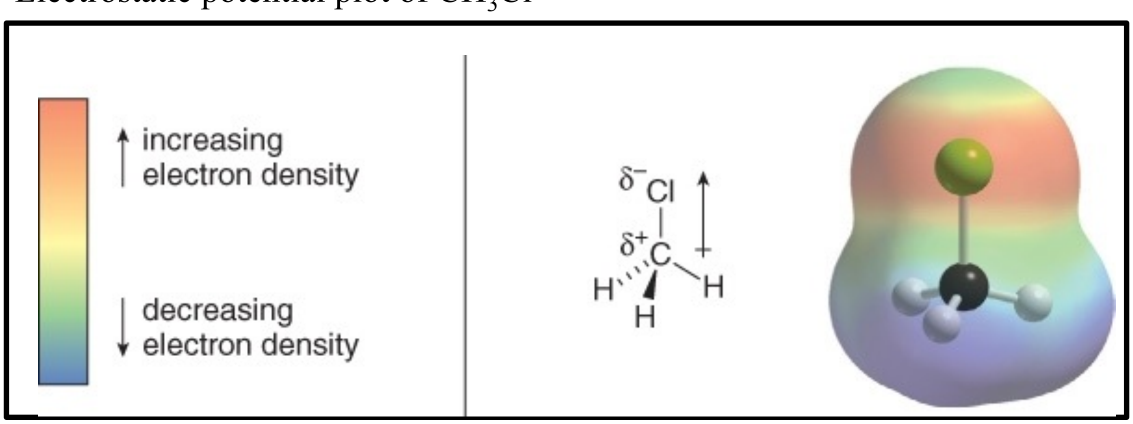






## Net Dipole of Molecules

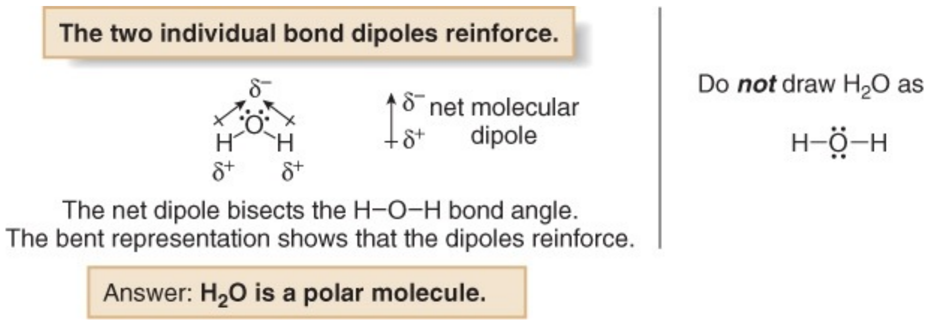
1. Use electronegativity differences to identify dipole directions of all of the polar bonds.
2. Decide if individual dipoles cancel or reinforce each other in space.

Electrostatic potential plot of $CH_3Cl$



# Structure and Bonding: Polarity of Molecules

A polar molecule has either one polar bond, or two or more bond dipoles that reinforce each other. An example is water:




A nonpolar molecule has either no polar bonds, or two or more bond dipoles that cancel. An example is carbon dioxide: