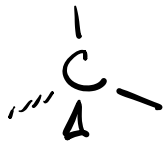
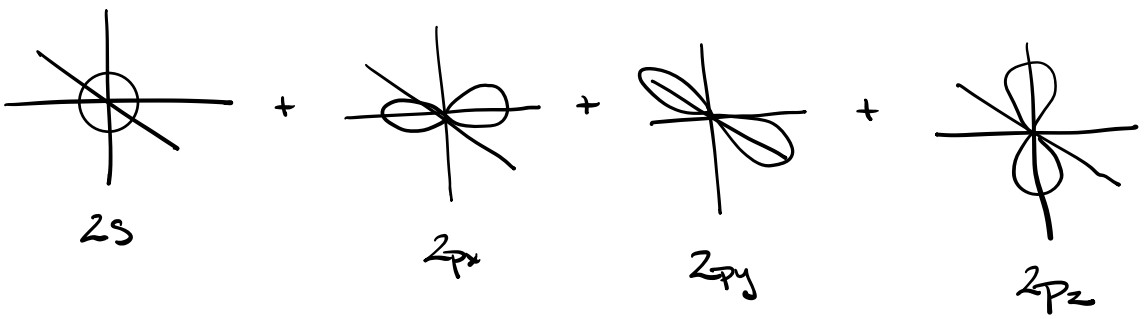
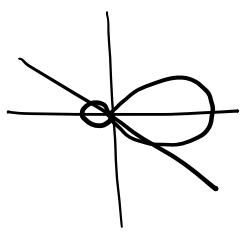
# Natural Bonding Theory

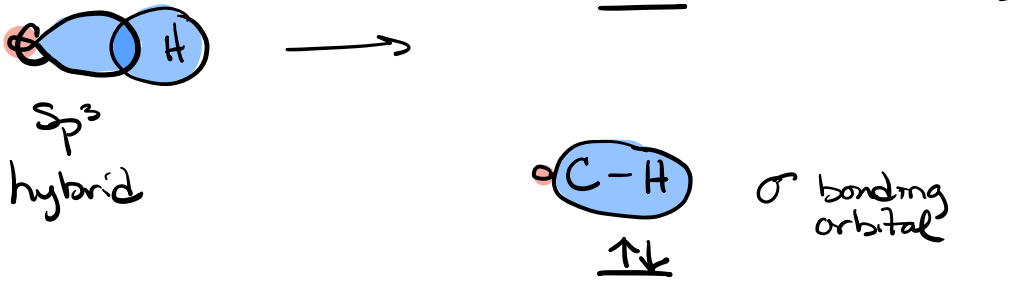
Linear Combination
atomic orbitals → hybrid orbitals → Bonding Orbital / Molecular Orbital
weighted additions

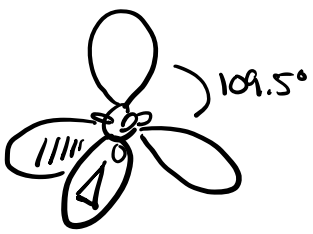

Tetrahedral




= 4 hybrid orbitals


$Sp^3$ hybrid

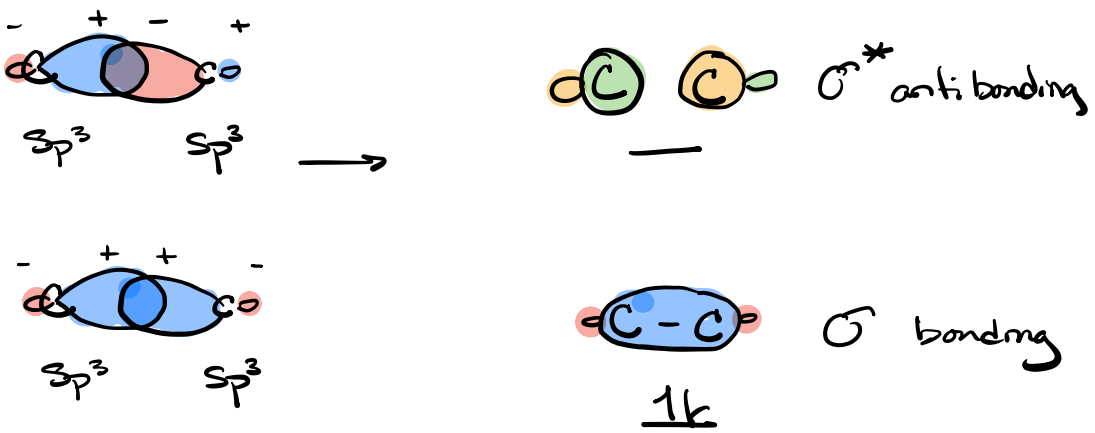



Tetrahedral = "$sp^3$ hybridized"

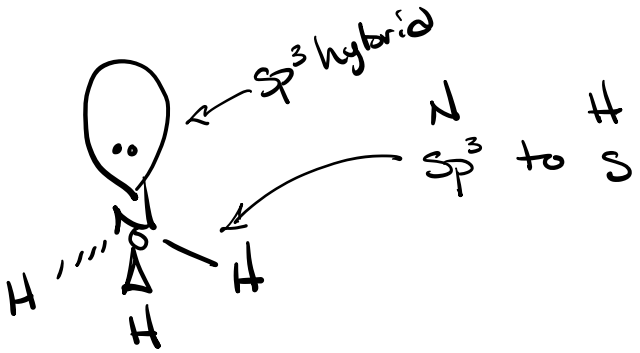
more important

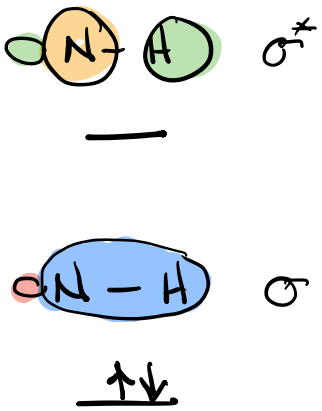
4 $sp^3$ hybrid orbitals



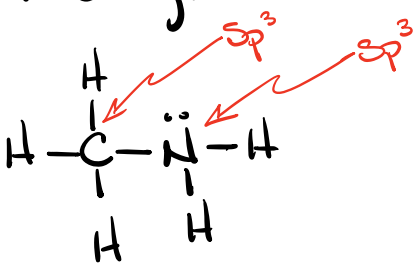
Tetrahedral = $sp^3$ hybridized

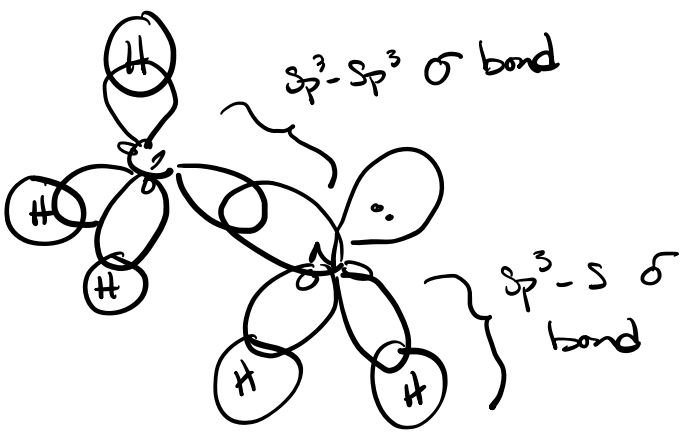
"Trigonal Pyramidal"



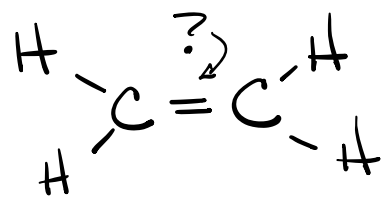




Methyl amine



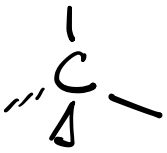



Trigonal Planar



What is the hybridization?
How do we get 120° bond angle?

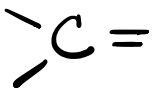
Alkene
Ethylene



needed 4 hybrids

$S + P_x + P_y + P_z = 4 @ Sp^3$

$\frac{1}{4}S + \frac{3}{4}P$

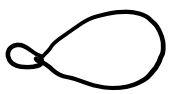


Need to bond to 3 things (atoms)
need 3 hybrids

$S + P_x + P_y + P_z$ ~~$P_z$~~

3 hybrids @ $Sp^2$

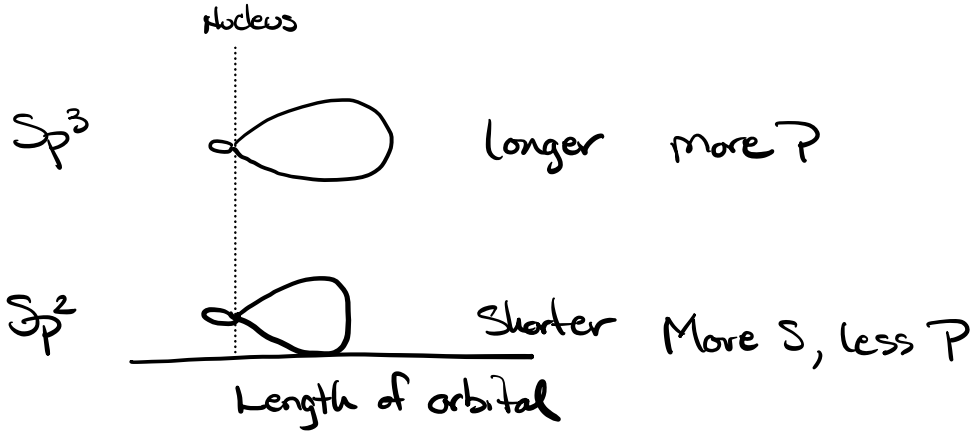
$\frac{1}{3}S + \frac{2}{3}P$



$Sp^2$

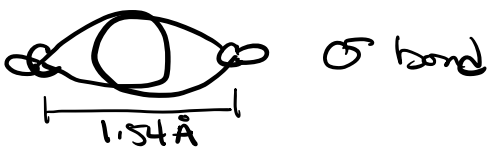
more S character
& less p character

# Comparing $sp^2$ to $sp^3$



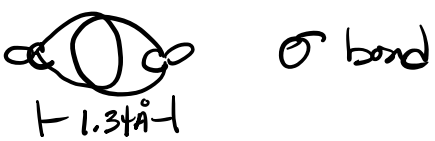

C–C

$sp^3 - sp^3$

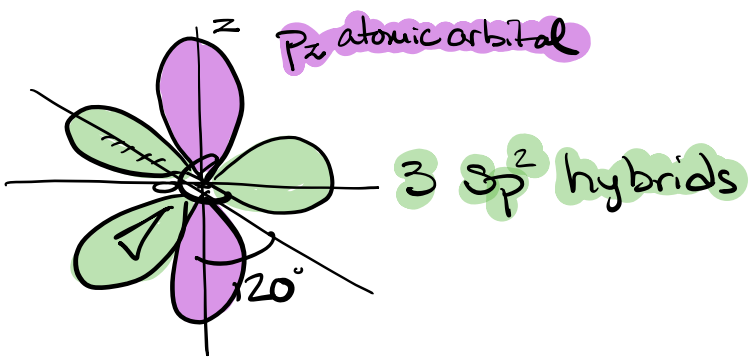


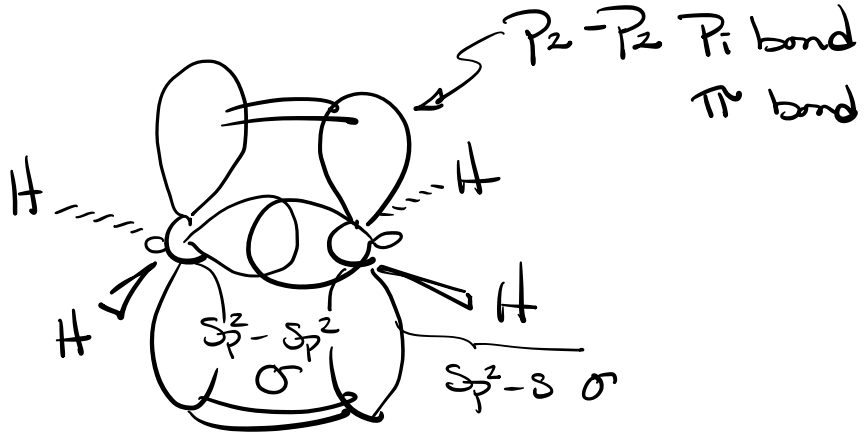

C–C

$sp^2$ $sp^2$

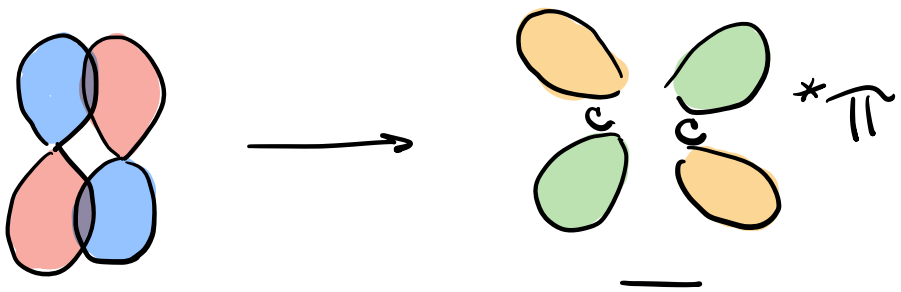


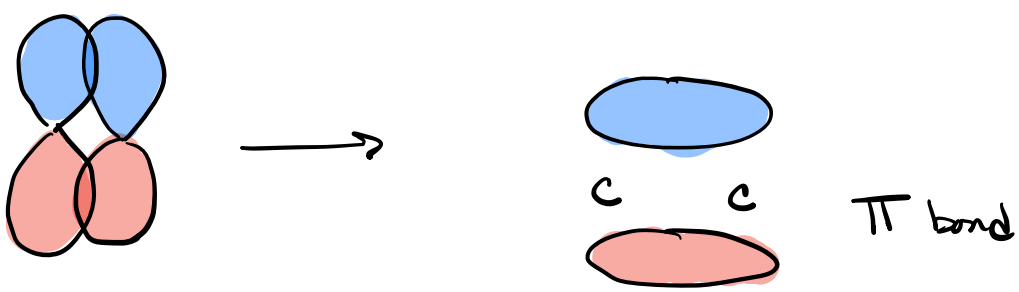

much shorter bond
due to shorter orbitals






## $\pi$ bond

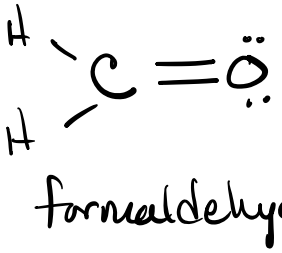


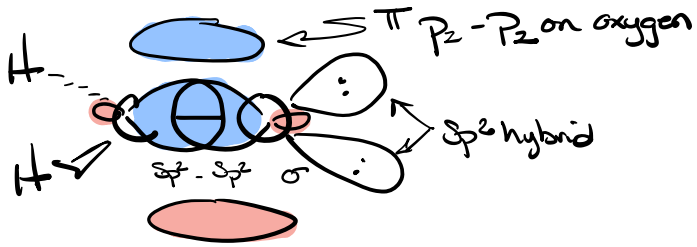

$\uparrow\downarrow$

$e^-$ density above & below atoms


$e^-$ density in between atom




formaldehyde



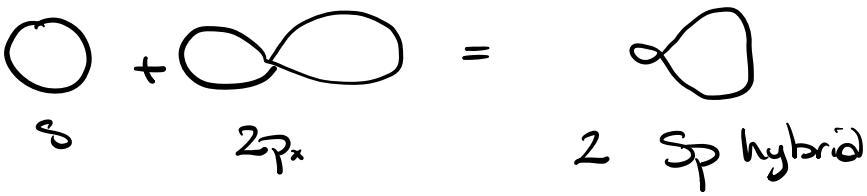

## Linear Geometry Alkynes

$H-C\equiv C-H$

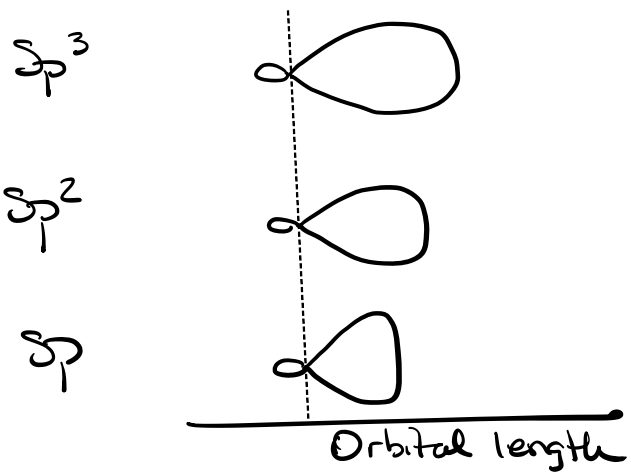
180°

$-C\equiv$

Bonded to 2 things
= 2 hybrids




$2p_y$ & $2p_z$ unused $\Rightarrow$ π bonds

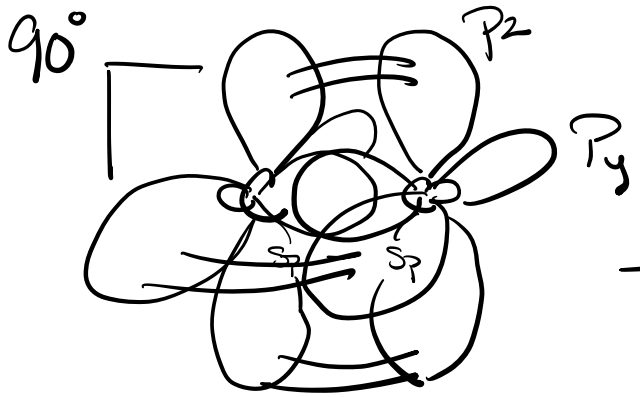



$C_{sp^3}-C_{sp^3}$ 1.54 Å

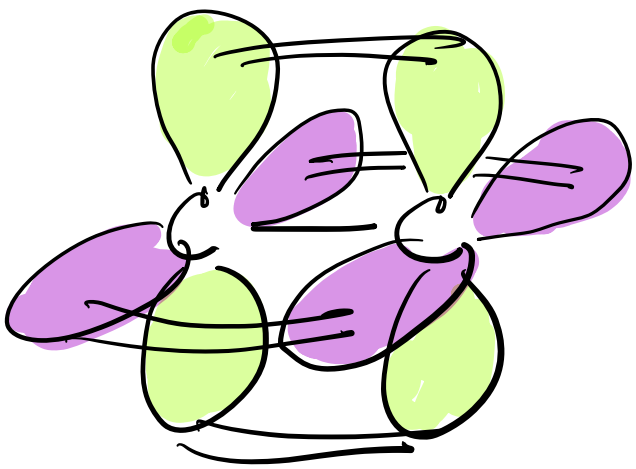
$C_{sp^2}=C_{sp^2}$ 1.34 Å

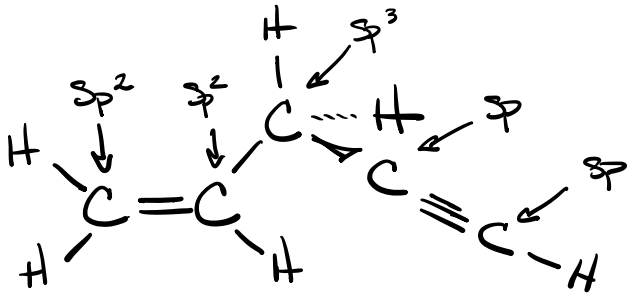
$C_{sp}\equiv C_{sp}$ 1.20 Å

Because the hybrid orbitals decrease in size from $sp^3 \rightarrow sp^2 \rightarrow sp$ - to the make the bond requires orbital overlap. Atoms must get closer to have required overlap for bond formation → bond gets shorter.

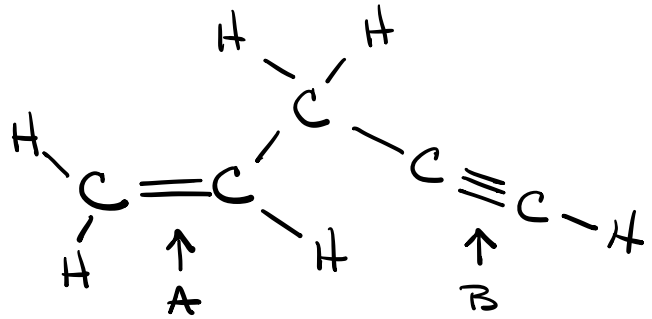


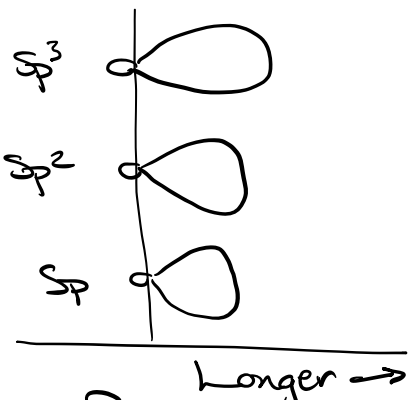

Two π bonds



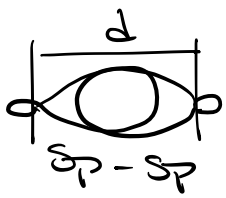


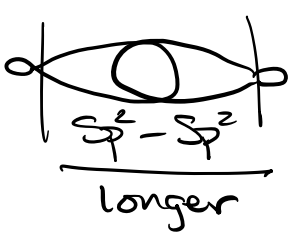

Give the hybridization of each carbon.



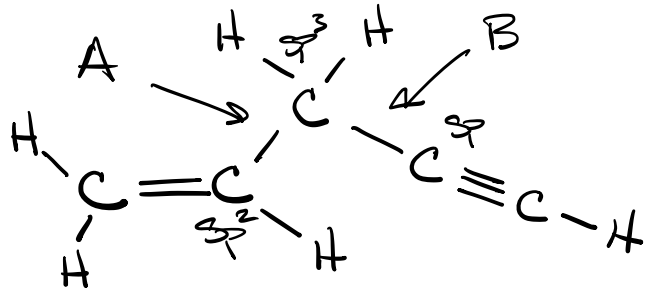

which bond is longer A or B ?




- $sp^3 > sp^2 > sp$
- Shorter orbitals require atoms to get closer for orbital overlap to make bond
- sp - sp Shortest bond

$\Rightarrow$ $sp^2$-$sp^2$ Longest | A |




Which bond is longer, A or B ?

A

$Sp^2 - Sp^3$ ⟸ longer orbital ⇒ Longer bond

↑ Longer than Sp

Same

B

$Sp - Sp^3$

↑ shortest