## HYBRIDIZATION

Hybridization is the mixing together of "atomic orbitals" (i.e., s-, p-) to form new, *hybridized* atomic orbitals. These new, hybridized, atomic orbitals overlap to form  $\sigma$  and  $\pi$  bonds. Carbon, oxygen and nitrogen valence atomic orbitals hybridize to form sp3, sp2 or sp hybridized orbitals. For *neutral (no formal charge)* C, O, and N atoms, the following guidelines in the table below can be used to predict the hybridization of these atoms in organic molecules.

	CARBON			
	Valence atomic orbitals	Hybridized atomic orbitals	Bonding Pattern, geometry and bond angles in molecules	
sp3	<b>2s + 2px + 2py + 2pz</b> All <u>four</u> of carbon's valence orbitals mix to form four new hybridized orbitals	sp3 + sp3 + sp3 + sp3 Four new, degenerate (equal energy) orbitals are generated after hybridization. Each orbital is used to form a sigma bond	(methane) (methane) Tetrahedral geometry(Td) 109° bond angles Four σ bonds	
sp2	$2s + 2px + 2py + 2pz$ $\frac{Three}{orbitals} of carbon's four valence}{orbitals} mix(in box) to form three new hybridized orbitals. The unhbridized p-orbital is used for \pi bonding$	sp2 + sp2 + sp2 + p Three new degenerate orbitals are formed after hybridization. The p orbital remains unhybridized. The sp2 orbitals are used to form $\sigma$ bonds and the p orbital is used to form a $\pi$ bond.	(ethylene) Trigonal planar geometry 120° bond angles Three $\sigma$ bonds, one $\pi$ bond	
sp	$2s + 2px$ $+ 2py + 2pz$ $\underline{Two}$ of carbon's four valence orbitals mix(in box) to form two new hybridized orbitals. The unhbridized p-orbitals are used for $\pi$ bonding	sp + sp + p + p Two new degenerate orbitals are generated after hybridization. The two p orbitals remain unhybridized. The sp orbitals are used to form $\sigma$ bonds and the p orbitals are used to form $\pi$ bonds.	(acetylene) Linear geometry 180° bond angles Two $\sigma$ bonds, two $\pi$ bonds	

NITROGEN			
	Valence atomic orbitals	Hybridized atomic orbitals	Bonding Pattern, geometry and bond angles in molecules
sp3	2s + 2px + 2py + 2pz All <u>four</u> of nitrogen's valence orbitals mix to form four new hybridized orbitals	sp3 + sp3 + sp3 + sp3 Four new, degenerate (equal energy) orbitals form after hybridization. Three of the sp3 orbitals are used to form $\sigma$ bonds and one is used for a lone pair.	(ammonia) Trigonal pyramidal Bond angles: 107° Three σ bonds and 1 lone pair
sp2	2s + 2px + 2py + 2pz <u>Three</u> of nitrogen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized p- orbital is used for $\pi$ bonding	sp2 + sp2 + sp2 + p Three new degenerate orbitals form after hybridization. The p orbital remains unhybridized. Two of the sp2 orbitals are used to form $\sigma$ bonds, one is used for a lone pair and the p orbital is used to form a $\pi$ bond.	formal damine) Bent geometry 120° bond angles Two σ bonds, one lone pair and one π bond
sp	$2s + 2px + 2py + 2pz$ $\frac{Two \ of \ nitrogen's \ four \ valence}{orbitals \ mix(in \ box) \ to \ form} two \ new \ hybridized \ orbitals.$ $The \ unhybridized \ p-orbitals \ are \ used \ for \ \pi \ bonding$	sp + sp + p + p Two new degenerate orbitals are generated after hybridization. The two p orbitals remain unhybridized. One of the sp orbitals is used to form a $\sigma$ bond and the other is used for the lone pair. The two unhybridized p orbitals are used to form two $\pi$ bonds.	(acetonitrile) Linear geometry 180° bond angles One $\sigma$ bond, one lone pair and two $\pi$ bonds

	OXYGEN			
	Valence atomic orbitals	Hybridized atomic orbitals	Bonding Pattern, geometry and bond angles in molecules	
sp3	2s + 2px + 2py + 2pz All four of oxygen's valence orbitals mix to form four new hybridized orbitals	sp3 + sp3 + sp3 + sp3 Four new orbitals form after hybridization. Two of the sp3 orbitals are used to form $\sigma$ bonds and two are used for two lone pairs.	(dimethylether) Bent 104° bond angles Two σ bonds and 2 lone pairs	
sp2	2s + 2px + 2py + 2pz Three of oxygen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized p-orbital is used for $\pi$ bonding	sp2 + sp2 + sp2 + p Three new orbitals form after hybridization. The p orbital remains unhybridized. One of the sp2 orbitals are used to form $\sigma$ bond, two are used for lone pairs and the p orbital is used to form a $\pi$ bond.	formaldehyde) (formaldehyde) Linear geometry 180°bond angles Two σ bonds, one lone pair and one π bond	

## Example molecules:



Н

'n

H,

Н

`\_\_\_\_=



NH || C

H7

`н





CH<sub>3</sub>

н—с≡с—н

 $CH_3 - C \equiv N$ 

For charged atoms (those with formal charge), bonding patterns for specifically hybridized atoms is different. Charged atoms are encountered during chemical reactions as reaction intermediates.

CHARGED CARBON ATOMS			
	Valence atomic orbitals	Hybridized atomic orbitals	Bonding Pattern, geometry and bond angles in molecules
$\begin{array}{c} m_{m_{m_{n_{n_{n_{n_{n_{n_{n_{n_{n_{n_{n_{n_{n_$	2s + 2px + 2py + 2pz Three of carbon's valence orbitals mix to form three new hybridized orbitals. One of the p orbitals remains unhybridized	sp2 + sp2 + sp2 + p Three new, orbitals are formed after hybridization. The three sp2 orbitals are used to form $\sigma$ bonds. The p orbital remains vacant (no electrons and is available to accept electrons from a nucleophile.)	Trigonal planar 120° bond angles Three $\sigma$ bonds and 1 vacant p-orbital
$ext{arbanion} 1s^22s^22p^3$ sp3	<b>2s + 2px + 2py + 2pz</b> All four of carbon's four valence orbitals mix to form four new hybridized orbitals.	sp3 + sp3 + sp3 + sp3 Four new degenerate orbitals form after hybridization. Three of the sp3 orbitals are used to form $\sigma$ bonds, one is used for a lone pair.	Trigonal pyramidal 107° bond angles Three σ bonds and one lone pair

CHARGED NITROGEN ATOMS				
Nitrogen atoms may commonly encounte	Nitrogen atoms may take on a positive charge or a negative charge in a reactive state. Positively charged N atoms are most commonly encountered when the nitrogen atom uses its lone pair to accept a proton (H) in an acid-base reaction. Negatively			
	Valence atomic orbitals	Hybridized atomic orbitals	Bonding Pattern, geometry and bond angles in molecules	
sp3	<b>2s + 2px + 2py + 2pz</b> All <u>four</u> of nitrogen's valence orbitals mix to form four new hybridized orbitals	sp3 + sp3 + sp3 + sp3 Four new, degenerate (equal energy) orbitals form after hybridization. All four of the sp3 orbitals are used to form $\sigma$ bonds.	$Tetrahedral$ $Bond \ angles: \ 109^{\circ}$ $Four \ \sigma \ bonds$	
⊖ N	<b>2s + 2px + 2py + 2pz</b> All <u>four</u> of nitrogen's valence orbitals mix to form four new hybridized orbitals	sp3 + sp3 + sp3 + sp3 Four new, degenerate (equal energy) orbitals form after hybridization. Two the sp3 orbitals are used to form $\sigma$ bonds and two are used for two lone pairs.	Bent geometry $104^{\circ}$ bond angles Two $\sigma$ bonds ; 2 lone pairs	
$ \begin{array}{c}                                     $	$2s + 2px + 2py + 2pz$ $\underline{Three} of nitrogen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized porbital is used for \pi bonding$	sp2 + sp2 + sp2 + p Three new degenerate orbitals form after hybridization. The p orbital is unhybridized. Three of the sp2 orbitals are used to form $\sigma$ bonds, and the p orbital is used to form a $\pi$ bond.	$Frigonal planar \\ 120^{\circ} bond angles \\ Three \ \sigma \ bonds; \ one \ \pi \ bond$	
c <sup>⊕</sup> sp	$2s + 2px + 2py + 2pz$ $\frac{Two}{of} nitrogen's four$ valence orbitals mix(in box) to form two new hybridized orbitals. The unhybridized p- orbitals are used for $\pi$ bonding	sp + sp + p + p Two new degenerate orbitals are generated after hybridization. The two p orbitals remain unhybridized. The sp orbitals are used to form $\sigma$ bonds. The two unhybridized p orbitals are used to form two $\pi$ bonds.	Linear 180° bond angles Two $\sigma$ bonds; two $\pi$ bonds	

CHARGED OXYGEN ATOMS			
Oxygen atoms may take on a positive charge or a negative charge in a reactive state. Positively charged O atoms (oxonium ion) are most commonly encountered when the oxygen atom uses one of its lone pairs to accept a proton (H) in an acid-catalyzed reaction. Negatively charged oxygen atoms (hydroxides or alkoxides) are formed under basic conditions			
	Valence atomic orbitals	Hybridized atomic orbitals	Bonding Pattern, geometry and bond angles in molecules
H I I I I I I I I I I I I I I I I I I I	<b>2s + 2px + 2py + 2pz</b> All <u>four</u> of oxygen's valence orbitals mix to form four new hybridized orbitals	sp3 + sp3 + sp3 + sp3 Four new, $sp3$ orbitals form after hybridization. Three of the $sp3$ orbitals are used for $\sigma$ bonds and one for a lone pair	Trigonal pyramidal Bond angles: 107° Three σbonds; one lone pair
	2s + 2px + 2py + 2pz	sp3 + sp3 + sp3 + sp3	
⊖ Ö. sp3	All <u>four</u> of oxygen's valence orbitals mix to form four new hybridized orbitals	Four new, sp3 orbitals form after hybridization. Three of the sp3 orbitals are used for lone pairs and one for a $\sigma$ bond.	One $\sigma$ bond ; 3 lone pairs
$ \begin{array}{c}                                     $	$2s + 2px + 2py + 2pz$ $\underline{Three} of oxygen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized p-orbital is used for \pi bonding$	sp2 + sp2 + sp2 + p Three new $sp2$ orbitals form after hybridization. The p orbital is unhybridized. Two of the $sp2$ orbitals are used to form $\sigma$ bonds, one is for a lone pair and the p orbital for a $\pi$ bond.	Figure Field Fi
c≞o sp	$2s + 2px + 2py + 2pz$ $\underline{Two} of oxygen's four$ valence orbitals mix(in box) to form two new hybridized orbitals. The unhybridized p- orbitals are used for $\pi$ bonding	sp + sp + p + p Two new sp orbitals are generated after hybridization. The two p orbitals remain unhybridized. The sp orbitals are used for one $\sigma$ bond and one lone pair. The two unhybridized p orbitals are	Einear One $\sigma$ bonds; one lone pair; two $\pi$ bonds