## 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 sp 3 , sp 2 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 | $2 s+2 p x+2 p y+2 p z$ <br> All four of carbon's valence orbitals mix to form four new hybridized orbitals | sp3 + sp3 + sp3 + sp3 <br> Four new, degenerate (equal energy) orbitals are generated after hybridization. Each orbital is used to form a sigma bond | (methane) <br> Tetrahedral geometry(Td) $109^{\circ}$ bond angles Four $\sigma$ bonds |
| sp2 | $2 s+2 p x+2 p y+2 p z$ <br> Three of carbon's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhbridized p-orbital is used for $\pi$ bonding | $\mathbf{s p 2}+\mathbf{s p} 2+\mathbf{s p} 2+\mathbf{p}$ <br> 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) <br> Trigonal planar geometry $120^{\circ}$ bond angles <br> Three $\sigma$ bonds, one $\pi$ bond |
| sp | $2 s+2 p x+2 p y+2 p z$ <br> 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 | $\mathbf{s p}+\mathbf{s p}+\mathbf{p}+\mathbf{p}$ <br> 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) <br> Linear geometry <br> $180^{\circ}$ bond angles <br> Two $\sigma$ bonds, two $\pi$ bonds |


| NITROGEN |  |  |  |
| :---: | :---: | :---: | :---: |
|  | Valence atomic orbitals | Hybridized atomic orbitals | Bonding Pattern, geometry and bond angles in molecules |
| sp3 | $2 s+2 p x+2 p y+2 p z$ <br> All four of nitrogen's valence orbitals mix to form four new hybridized orbitals | sp3 + sp3 + sp3 + sp3 <br> 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) <br> Trigonal pyramidal <br> Bond angles: $107^{\circ}$ <br> Three $\sigma$ bonds and 1 lone pair |
| sp2 | $2 s+2 p x+2 p y+2 p z$ <br> Three of nitrogen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized porbital is used for $\pi$ bonding | $\mathbf{s p} 2+\mathbf{s p} 2+\mathbf{s p} 2+\mathbf{p}$ <br> 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. | (formaldamine) Bent geometry $120^{\circ}$ bond angles <br> Two $\sigma$ bonds, one lone pair and one $\pi$ bond |
| sp | $2 s+2 p x+2 p y+2 p z$ <br> 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 | $\mathbf{s p}+\mathbf{s p}+\mathbf{p}+\mathbf{p}$ <br> 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) <br> Linear geometry $180^{\circ}$ bond angles <br> 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 | $2 s+2 p x+2 p y+2 p z$ <br> All four of oxygen's valence orbitals mix to form four new hybridized orbitals | sp3 + sp3 + sp3 + sp3 <br> 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 <br> $104^{\circ}$ bond angles <br> Two $\sigma$ bonds and 2 lone pairs |
| sp2 | $2 s+2 p x+2 p y+2 p z$ <br> 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 | $\mathbf{s p} 2+\mathbf{s p} 2+\mathbf{s p} 2+\mathbf{p}$ <br> 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) <br> Linear geometry <br> $180^{\circ}$ bond angles <br> Two $\sigma$ bonds, one lone pair and one $\pi$ bond |

## Example molecules:







$\mathrm{H}_{3}-\mathrm{C} \equiv \mathrm{N}$


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 |  |  |  |
| :---: | :--- | :--- | :--- |
|  | $\begin{array}{c}\text { Valence } \\ \text { atomic orbitals }\end{array}$ | $\begin{array}{c}\text { Hybridized } \\ \text { atomic orbitals }\end{array}$ | $\begin{array}{c}\text { Bonding Pattern, } \\ \text { geometry and bond } \\ \text { angles }\end{array}$ |
| in molecules |  |  |  |$]$

## CHARGED NITROGEN ATOMS

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 $(\mathrm{H})$ in an acid-base reaction. Negatively charged nitrogen atoms are much less common but may be generated during chemical reactions.

|  | Valence atomic orbitals | Hybridized atomic orbitals | Bonding Pattern, geometry and bond angles in molecules |
| :---: | :---: | :---: | :---: |
|  | $2 s+2 p x+2 p y+2 p z$ <br> All four of nitrogen's valence orbitals mix to form four new hybridized orbitals | $\mathbf{s p} 3+\mathbf{s p} 3+\mathbf{s p} 3+\mathbf{s p} 3$ <br> Four new, degenerate (equal energy) orbitals form after hybridization. All four of the sp3 orbitals are used to form $\sigma$ bonds. | Tetrahedral <br> Bond angles: $109^{\circ}$ <br> Four $\sigma$ bonds |
|  <br> sp3 | $2 s+2 p x+2 p y+2 p z$ <br> All four of nitrogen's valence orbitals mix to form four new hybridized orbitals | sp3 + sp3 + sp3 + sp3 <br> 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 <br> Two $\sigma$ bonds ; 2 lone pairs |
|  | $2 s+2 p x+2 p y+2 p z$ <br> Three of nitrogen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized porbital is used for $\pi$ bonding | $\mathbf{s p} 2+\mathrm{sp} 2+\mathrm{sp} 2+\mathbf{p}$ <br> Three new degenerate orbitals form after hybridization. The p orbital is unhybridized. <br> Three of the sp2 orbitals are used to form $\sigma$ bonds, and the $p$ orbital is used to form a $\pi$ bond. | Trigonal planar $120^{\circ}$ bond angles <br> Three $\sigma$ bonds; one $\pi$ bond |
| $\begin{aligned} &-\mathrm{C} \stackrel{\oplus}{\mathrm{~N}}- \\ & \mathbf{s p} \end{aligned}$ | $2 s+2 p x+2 p y+2 p z$ <br> 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 | $\mathbf{s p}+\mathbf{s p}+\mathbf{p}+\mathbf{p}$ <br> 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 <br> $180^{\circ}$ bond angles <br> 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 |
| :---: | :---: | :---: | :---: |
|  | $2 s+2 p x+2 p y+2 p z$ <br> All four of oxygen's valence orbitals mix to form four new hybridized orbitals | sp3 + sp3 + sp3 + sp3 <br> 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 <br> Bond angles: $107^{\circ}$ <br> Three $\sigma$ bonds; one lone pair |
|  <br> sp3 | $2 s+2 p x+2 p y+2 p z$ <br> All four of oxygen's valence orbitals mix to form four new hybridized orbitals | sp3 + sp3 + sp3 + sp3 <br> 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 |
|  | $2 s+2 p x+2 p y+2 p z$ <br> Three of oxygen's four valence orbitals mix(in box) to form three new hybridized orbitals. The unhybridized porbital is used for $\pi$ bonding | $\mathbf{s p 2}+\mathbf{s p} 2+\mathbf{s p} 2+\mathbf{p}$ <br> 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. | Bent <br> Two $\sigma$ bonds; one lone pair; one $\pi$ bond |
| $\begin{gathered} -\mathrm{C} \equiv \stackrel{\oplus}{\mathrm{O}} \\ \mathbf{s p} \end{gathered}$ | $2 s+2 p x+2 p y+2 p z$ <br> Two of oxygen's four valence orbitals mix(in box) to form two new hybridized orbitals. The unhybridized porbitals are used for $\pi$ bonding | $\mathbf{s p}+\mathbf{s p}+\mathbf{p}+\mathbf{p}$ <br> 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 used to form two $\pi$ bonds. | Linear <br> One $\sigma$ bonds; one lone pair; two $\pi$ bonds |

