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.

<table>
<thead>
<tr>
<th>CARBON</th>
<th>Valence atomic orbitals</th>
<th>Hybridized atomic orbitals</th>
<th>Bonding Pattern, geometry and bond angles in molecules</th>
</tr>
</thead>
</table>
| sp$^3$ | $2s + 2px + 2py + 2pz$  | sp$^3$ + sp$^3$ + sp$^3$ + sp$^3$ | (methane)  
Tetrahedral geometry (Td)  
$109^\circ$ bond angles  
Four $\sigma$ bonds |
| sp$^2$ | $2s + 2px + 2py + 2pz$  | sp$^2$ + sp$^2$ + sp$^2$ + p | (ethylene)  
Trigonal planar geometry  
$120^\circ$ bond angles  
Three $\sigma$ bonds, one $\pi$ bond |
| sp     | $2s + 2px + 2py + 2pz$  | sp + sp + p + p           | (acetylene)  
Linear geometry  
$180^\circ$ bond angles  
Two $\sigma$ bonds, two $\pi$ bonds |
<table>
<thead>
<tr>
<th>NITROGEN</th>
<th>Valence atomic orbitals</th>
<th>Hybridized atomic orbitals</th>
<th>Bonding Pattern, geometry and bond angles in molecules</th>
</tr>
</thead>
<tbody>
<tr>
<td>sp³</td>
<td>$2s + 2px + 2py + 2pz$</td>
<td>$sp³ + sp³ + sp³ + sp³$</td>
<td>(ammonia) Trigonal pyramidal Bond angles: 107° Three $\sigma$ bonds and 1 lone pair</td>
</tr>
<tr>
<td></td>
<td>All four of nitrogen's valence orbitals mix to form four new hybridized orbitals</td>
<td>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.</td>
<td></td>
</tr>
<tr>
<td>sp²</td>
<td>$2s + 2px + 2py + 2pz$</td>
<td>$sp² + sp² + sp² + p$</td>
<td>(formaldamine) Bent geometry 120° bond angles Two $\sigma$ bonds, one lone pair and one $\pi$ bond</td>
</tr>
<tr>
<td></td>
<td>Three of nitrogen's four valence orbitals mix (in box) to form three new hybridized orbitals. The unhybridized p-orbital is used for $\pi$ bonding</td>
<td>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.</td>
<td></td>
</tr>
<tr>
<td>sp</td>
<td>$2s + 2px + 2py + 2pz$</td>
<td>$sp + sp + p + p$</td>
<td>(acetonitrile) Linear geometry 180° bond angles One $\sigma$ bond, one lone pair and two $\pi$ bonds</td>
</tr>
<tr>
<td></td>
<td>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</td>
<td>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.</td>
<td></td>
</tr>
</tbody>
</table>
# OXYGEN

<table>
<thead>
<tr>
<th>Valence atomic orbitals</th>
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</tr>
</thead>
</table>
| **sp³** 2s + 2px + 2py + 2pz | **sp³ + sp³ + sp³ + sp³** | (dimethylether)  
Bent  
104° bond angles  
Two σ bonds and 2 lone pairs |
| All four of oxygen’s valence orbitals mix to form four new hybridized orbitals | Four new orbitals form after hybridization. Two of the sp³ orbitals are used to form σ bonds and two are used for two lone pairs. | |
| **sp²** 2s + 2px + 2py + 2pz | **sp² + sp² + sp² + p** | (formaldehyde)  
Linear geometry  
180° bond angles  
Two σ bonds, one lone pair and one π bond |
| Three of oxygen’s four valence orbitals mix (in box) to form three new hybridized orbitals. The unhybridized p-orbital is used for π bonding | Three new orbitals form after hybridization. The p orbital remains unhybridized. One of the sp² orbitals are used to form σ bond, two are used for lone pairs and the p orbital is used to form a π bond. | |

**Example molecules:**

![Methane](image1.png)

![Ethylene](image2.png)

![Formaldehyde](image3.png)

![Dimethylether](image4.png)

![Formamide](image5.png)

![Methylacetylene](image6.png)
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.

<table>
<thead>
<tr>
<th>CHARGED CARBON ATOMS</th>
<th>Valence atomic orbitals</th>
<th>Hybridized atomic orbitals</th>
<th>Bonding Pattern, geometry and bond angles in molecules</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="carbocation" /></td>
<td>1s² 2s² 2p¹ sp²</td>
<td>2s + 2px + 2py + 2pz</td>
<td>sp² + sp² + sp² + p</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Three of carbon's valence orbitals mix to form three new hybridized orbitals. One of the p orbitals remains unhybridized</td>
<td>Three new, orbitals are formed after hybridization. The three sp² orbitals are used to form σ bonds. The p orbital remains vacant (no electrons and is available to accept electrons from a nucleophile.)</td>
</tr>
<tr>
<td><img src="image2" alt="carbanion" /></td>
<td>1s² 2s² 2p³ sp³</td>
<td>2s + 2px + 2py + 2pz</td>
<td>sp³ + sp³ + sp³ + sp³</td>
</tr>
<tr>
<td></td>
<td></td>
<td>All four of carbon's four valence orbitals mix to form four new hybridized orbitals.</td>
<td>Four new degenerate orbitals form after hybridization. Three of the sp³ orbitals are used to form σ bonds, one is used for a lone pair.</td>
</tr>
</tbody>
</table>

Trigonal planar 120° bond angles
Three σ bonds and 1 vacant p-orbital

Trigonal pyramidal 107° bond angles
Three σ bonds and one lone pair
### 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 (H) in an acid-base reaction. Negatively charged nitrogen atoms are much less common but may be generated during chemical reactions.

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</table>
| ![sp3](image)  
2s + 2px + 2py + 2pz  
All four 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 σ bonds. | Tetrahedral  
Bond angles: 109°  
Four σ bonds |
| ![sp3](image)  
2s + 2px + 2py + 2pz  
All four 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 σ bonds and two are used for two lone pairs. | Bent geometry  
104° bond angles  
Two σ bonds; 2 lone pairs |
| ![sp2](image)  
2s + 2px + 2py + 2pz  
Three of nitrogen's four valence orbitals mix (in box) to form three new hybridized orbitals. The unhybridized p-orbital is used for π 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 σ bonds, and the p orbital is used to form a π bond. | Trigonal planar  
120° bond angles  
Three σ bonds; one π bond |
| ![sp](image)  
2s + 2px + 2py + 2pz  
Two of nitrogen's four valence orbitals mix (in box) to form two new hybridized orbitals. The unhybridized p-orbitals are used for π 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 σ bonds. The two unhybridized p orbitals are used to form two π bonds. | Linear  
180° bond angles  
Two σ bonds; two π bonds |
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.

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<tr>
<td>sp³</td>
<td>sp³ + sp³ + sp³ + sp³</td>
<td>Trigonal pyramidal Bond angles: 107° Three σ bonds; one lone pair</td>
</tr>
<tr>
<td>sp³</td>
<td>sp³ + sp³ + sp³ + p</td>
<td>Bent Two σ bonds; one lone pair; one π bond</td>
</tr>
<tr>
<td>sp³</td>
<td>sp + sp + p + p</td>
<td>Linear One σ bonds; one lone pair; two π bonds</td>
</tr>
</tbody>
</table>

All four of oxygen's valence orbitals mix to form four new hybridized orbitals.

Three of oxygen's four valence orbitals mix (in box) to form three new hybridized orbitals. The unhybridized p-orbital is used for π bonding.

Three new sp² orbitals form after hybridization. The p orbital is unhybridized. Two of the sp² orbitals are used to form σ bonds, one is for a lone pair and the p orbital for a π bond.

Two new sp orbitals are generated after hybridization. The two p orbitals remain unhybridized. The sp orbitals are used for one σ bond and one lone pair. The two unhybridized p orbitals are used to form two π bonds.