Worksheet 16 - Hybridization

When atoms bond to form molecules, they use molecular orbitals. These are formed through the hybridization of the atomic orbitals that we have already discussed, s, p, and d orbitals.

The hybridized molecular orbitals have different shapes and energy levels than the atomic orbitals. The number of molecular orbitals created by hybridization depends on the number of atomic orbitals that are mixed to form them.

In forming \( sp^3 \) hybridized orbitals, four atomic orbitals are mixed, one s and three p. The energy diagram for this process is shown below. The hybridized orbitals are higher in energy than the s orbital, but lower in energy than the p orbitals, following Hund's rule.

\[
\begin{array}{cccccc}
\text{energy} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \text{hybridization} \\
\text{atomic orbitals} & s & p & & & \text{hybridized orbitals} \quad sp^3
\end{array}
\]

Carbon has 4 valence electrons. Add these electrons to the atomic and molecular orbitals. This hybridization gives tetrahedral geometry.

With this hybridization, C will form four equivalent \( \sigma \) bonds.

Draw a similar energy diagram for \( sp^3 \) hybridized oxygen.

\[
\begin{array}{cccccc}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \text{hybridization} \\
\text{atomic orbitals} & s & p & & & \text{hybridized orbitals} \quad sp^3
\end{array}
\]

How many \( \sigma \) bonds will be formed? 2

How are the other \( sp^3 \) orbitals used? \( \text{low pairs of } C^- \)

Do the same for \( sp^3 \) hybridized nitrogen.

\[
\begin{array}{cccccc}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \text{hybridization} \\
\text{atomic orbitals} & s & p & & & \text{hybridized orbitals} \quad sp^3
\end{array}
\]

3 \( \sigma \) bonds, 1 \( \text{low pair} \)
In some Lewis structures, there are only three equivalent bonds formed. To create three equivalent hybridized orbitals, mix three atomic orbitals.

Draw and name the orbitals formed in this hybridization, then add the electrons for sulfur. Since the hybridized orbitals are close in energy, every orbital is filled with one electron before electrons are paired.

The hybridized orbitals will form $1 \sigma$ bond(s).

The unhybridized orbital will form $1 \pi$ bond(s).

There will be 2 lone pair(s).

This hybridization gives trigonal planar geometry.

In linear molecules, like CO$_2$, the central atom has only two equivalent bonding orbitals. Draw the energy levels and name the orbitals formed in this hybridization.

Fill in the electrons for carbon and determine the number and type of bonds formed.

In CO$_2$, determine the hybridization of the oxygen atoms. Complete the energy diagram for the oxygens. Draw the structure of CO$_2$. 
In atoms with n=3 or larger, the d orbitals can also be hybridized. In molecules with five molecular orbitals, five atomic orbitals are mixed:

\[ d + s + p + p + p \]

This will give trigonal bipyramidal geometry and is called \( dsp^3 \) hybridization.

Finally, molecules with octahedral geometry, will have 6 molecular orbitals. This hybridization is called \( d^2 sp^3 \).

Shown below is a portion of the chart from Worksheet 14. Fill in the hybridization for each of the compounds.

<table>
<thead>
<tr>
<th>compound</th>
<th>bonds</th>
<th>lone pairs</th>
<th>geometry</th>
<th>shape</th>
<th>hybridization</th>
</tr>
</thead>
<tbody>
<tr>
<td>SF₆</td>
<td>6</td>
<td>0</td>
<td>octahedral</td>
<td>octahedral</td>
<td>( d^2 sp^3 )</td>
</tr>
<tr>
<td>NH₃</td>
<td>3</td>
<td>1</td>
<td>tetrahedral</td>
<td>trigonal pyramidal</td>
<td>( sp^3 )</td>
</tr>
<tr>
<td>ICl₄⁻</td>
<td>4</td>
<td>2</td>
<td>octahedral</td>
<td>square planar</td>
<td>( d^2 sp^3 )</td>
</tr>
<tr>
<td>CF₄</td>
<td>4</td>
<td>0</td>
<td>tetrahedral</td>
<td>tetrahedral</td>
<td>( sp^3 )</td>
</tr>
<tr>
<td>SO₃</td>
<td>3</td>
<td>0</td>
<td>trigonal planar</td>
<td>trigonal planar</td>
<td>( sp^2 )</td>
</tr>
<tr>
<td>SF₄</td>
<td>4</td>
<td>1</td>
<td>trigonal bipyramidal</td>
<td>seesaw</td>
<td>( dsp^3 )</td>
</tr>
<tr>
<td>CO₂</td>
<td>2</td>
<td>0</td>
<td>linear</td>
<td>linear</td>
<td>( sp )</td>
</tr>
<tr>
<td>H₂O</td>
<td>2</td>
<td>2</td>
<td>tetrahedral</td>
<td>V-shaped</td>
<td>( sp^3 )</td>
</tr>
<tr>
<td>NO₂⁻</td>
<td>2</td>
<td>1</td>
<td>trigonal planar</td>
<td>V-shaped</td>
<td>( sp^2 )</td>
</tr>
</tbody>
</table>
Fill in the chart below and then complete the Lewis structures for the molecules shown below and fill in those charts.

<table>
<thead>
<tr>
<th>element</th>
<th>Lewis symbol</th>
<th># bonds</th>
<th># lone pairs</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>( \cdot \cdot \cdot )</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>N</td>
<td>( \cdot \cdot \cdot )</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>( \cdot \cdot \cdot )</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>O</td>
<td>( \cdot \cdot \cdot )</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Halogen</td>
<td>( \cdot \cdot \cdot )</td>
<td>1</td>
<td>3</td>
</tr>
</tbody>
</table>

\[
\begin{aligned}
H_3^+ : O^- & \quad \sigma \text{ bonds} \quad 7 \\
H - C - C - O - H & \quad \pi \text{ bonds} \quad 1 \\
\text{acetic acid}
\end{aligned}
\]

\[
\begin{aligned}
H - C = C - C = N & \quad \sigma \text{ bonds} \quad 6 \\
H' & \quad \pi \text{ bonds} \quad 3 \\
\text{acylonitrile}
\end{aligned}
\]

\[
\begin{aligned}
H - C - N - C - N - C - N - C - N & \quad \sigma \text{ bonds} \quad 25 \\
H' & \quad \pi \text{ bonds} \quad 4 \\
\text{caffeine}
\end{aligned}
\]
Which atom carries the formal negative charge? (e)

How many $\pi$ and $\sigma$ bonds are present? (d)

How many resonance structures and label the hybridization of each oxygen. (c)

Label the hybridization around each carbon. (b)

Draw the Lewis structure and all resonance forms. (a)

Which of these rings are planar? (j)

How many $\pi$ bonds are there in total? (e)

How many $\sigma$ bonds are there in total? (d)

How many oxygens are $sp^3$ hybridized? (c)

How many nitrogens are $sp^3$ hybridized? (b)

How many carbons are $sp^3$ hybridized? (a)