Hybrid Orbitals

<table>
<thead>
<tr>
<th>HYBRID ORBITALS</th>
<th>NUMBER OF ORBITALS</th>
<th>Electron Domain Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>sp</td>
<td>2</td>
<td>linear</td>
</tr>
<tr>
<td>sp²</td>
<td>3</td>
<td>trigonal planar</td>
</tr>
<tr>
<td>sp³</td>
<td>4</td>
<td>tetrahedral</td>
</tr>
<tr>
<td>sp²d</td>
<td>4</td>
<td>square planar</td>
</tr>
<tr>
<td>sp³d</td>
<td>5</td>
<td>trigonal bipyramidal</td>
</tr>
<tr>
<td>sp³d²</td>
<td>6</td>
<td>octahedral</td>
</tr>
</tbody>
</table>

EXERCISES

A. Consider the molecule BeH₂.

1) Show the electronic structure of beryllium’s valence shell. Use arrows to represent the electrons contained in each orbital.

Be

\[ \begin{array}{c}
2s \\
\text{_____} \\
\text{_____} \\
2p \\
\text{_____} \\
\text{_____} \\
\end{array} \]

2) How many covalent bonds does the Be atom form with the H atoms?

3) Therefore, the beryllium atom should provide how many half-filled orbitals.

4) This is accomplished by creating a pair of hybrids and placing electron(s) in each of them. Show this in the following diagram, using up arrows (↑) to represent beryllium’s electrons. Label the orbitals:

Be*

\[ \begin{array}{c}
\text{_____} \\
\text{_____} \\
\text{_____} \\
\text{_____} \\
\text{_____} \\
\end{array} \]

5) Show the orbital diagram for the beryllium atom in the BeH₂ molecule, using down arrows (↓) to represent electrons from hydrogen:

Be*

\[ \begin{array}{c}
\text{_____} \\
\text{_____} \\
\text{_____} \\
\text{_____} \\
\text{_____} \\
\end{array} \]

6) What electron domain (ED) geometry does this molecule have?

B. Consider the molecule CH₄.

1) Show the electronic structure of carbon’s valence shell. Use arrows to represent the electrons contained in each orbital.

C

\[ \begin{array}{c}
2s \\
\text{_____} \\
\text{_____} \\
2p \\
\text{_____} \\
\text{_____} \\
\end{array} \]
2) How many covalent bonds does the C atom form with the H atoms?

3) Therefore, the carbon atom should provide ______ half-filled orbitals.

4) This is accomplished by creating four ______ hybrids and placing _____ electron(s) in each of them. Show this in the following diagram, using up arrows to represent carbon’s electrons. Label the orbitals:

   C* _____ _____ _____ _____

5) Show the orbital diagram for the carbon atom in the CH₄ molecule, using down arrows to represent electrons from hydrogen:

   C* _____ _____ _____ _____

6) What electron domain (ED) geometry does this molecule have?

C. Consider the molecule SF₆.

1) Show the electronic structure of sulphur’s valence shell. Use arrows to represent the electrons contained in each orbital.

   S 3s _____ _____ _____ 3p _____ _____ _____ 3d _____ _____

2) How many covalent bonds does the S atom form with the F atoms?

3) Therefore, the sulphur atom should provide ______ half-filled orbitals.

4) This is accomplished by creating six _____ hybrids and placing _____ electron(s) in each of them. Show this in the following diagram, using up arrows to represent sulphur’s electrons. Label the orbitals:

   S* _____ _____ _____ _____ _____ _____

5) Show the orbital diagram for the sulphur atom in the SF₆ molecule, using down arrows to represent electrons from fluorine:

   S* _____ _____ _____ _____ _____ _____

6) What electron domain (ED) geometry does this molecule have?

D. Consider the molecule SeF₄.

1) Show the electronic structure of selenium’s valence shell, ignoring the 3d orbitals, which are not involved in bonding in this molecule. Use arrows to represent the electrons contained in each orbital.
Se  
\[ 4s \quad 4p \quad 4d \]

2) How many covalent bonds does the Se atom form with the F atoms?

3) Therefore, the selenium atom should provide \( \text{how many?} \) half-filled orbitals.

4) This is accomplished by creating \( \text{sp} \) hybrids, placing \( \text{electron(s)} \) in four of them, and leaving \( \text{lone pair(s)} \) of electrons. Show this in the following diagram, using arrows to represent selenium’s electrons. Label the orbitals:

\[
\text{Se*} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_}
\]

5) Show the orbital diagram for the selenium atom in the SeF\(_4\) molecule, using darker arrows (or arrows in another colour) to represent electrons from fluorine:

\[
\text{Se*} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_} \quad \underline{\_\_\_\_}
\]

6) What electron domain (ED) geometry does this molecule have?

7) What is molecular geometry of this molecule?

**SOLUTIONS**

**A.**

\[
\begin{align*}
\text{Se} & \quad \begin{array}{c}
\text{Se}\rlap{^*} \\
1 \text{ electron;}
\end{array} \\
\text{Be} & \quad \begin{array}{c}
\text{Be}\rlap{^*} \\
1 \text{ electron;}
\end{array} \\
\text{Be} & \quad \begin{array}{c}
\text{Be}\rlap{^*} \\
2 \text{ sp hybrids; 1 electron;}
\end{array}
\end{align*}
\]

\[
\begin{align*}
\text{Be} & \quad \text{linear} \\
\text{Be} & \quad \text{linear}
\end{align*}
\]

**B.**

\[
\begin{align*}
\text{Se} & \quad \begin{array}{c}
\text{Se} \\
1 \text{ electron;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids; 1 electron;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids; 1 electron;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids; 1 electron;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids; 1 electron;}
\end{array}
\end{align*}
\]

\[
\begin{align*}
\text{C} & \quad \text{tetrahedral} \\
\text{C} & \quad \text{tetrahedral}
\end{align*}
\]

**C.**

\[
\begin{align*}
\text{Se} & \quad \begin{array}{c}
\text{Se} \\
1 \text{ electron;}
\end{array} \\
\text{S} & \quad \begin{array}{c}
\text{S} \\
6 \text{ sp\(^3\)d\(^2\) hybrids;}
\end{array} \\
\text{S} & \quad \begin{array}{c}
\text{S} \\
6 \text{ sp\(^3\)d\(^2\) hybrids;}
\end{array} \\
\text{S} & \quad \begin{array}{c}
\text{S} \\
6 \text{ sp\(^3\)d\(^2\) hybrids;}
\end{array}
\end{align*}
\]

\[
\begin{align*}
\text{S} & \quad \text{octahedral} \\
\text{S} & \quad \text{octahedral}
\end{align*}
\]

**D.**

\[
\begin{align*}
\text{Se} & \quad \begin{array}{c}
\text{Se} \\
1 \text{ electron; 1 lone pair;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids;}
\end{array} \\
\text{C} & \quad \begin{array}{c}
\text{C} \\
4 \text{ sp\(^3\) hybrids;}
\end{array}
\end{align*}
\]

\[
\begin{align*}
\text{C} & \quad \text{trigonal bipyramidal} \\
\text{C} & \quad \text{trigonal bipyramidal}
\end{align*}
\]