Unit 3 - Chemical Bonding:  
Molecular Structure  
Chapter 9

9.1 Determine the geometric arrangement of atoms in a molecule.  
[Readings 9.1 - 9.2 Problems 1-5, 56, 57, 58, 59, & 60]

Molecular Geometry & VSEPR  
Like charges repel, unlike charges attract.  
Electron pairs tend to get as close to the nucleus as possible while simultaneously getting as far from other pairs as possible.  
Electrons act in pairs because orbitals can assimilate pairs of electrons.  
These principles can be used to determine the geometry of a molecule.
2, 3, 4, 5, and 6 electron pairs and their geometries

**CO₂**

Lewis Structure:

Areas of charge density: 2

Geometry: Linear

**BF₃**

Lewis Structure:

Areas of charge density: 3

Geometry: Triangular Planar

Trigonal Planar
**CH$_4$**

Lewis Structure:

Areas of charge density: 4

Geometry: Tetrahedral

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**PCl$_5$**

Lewis Structure:

Areas of charge density: 5

Geometry: Triangular Bipyramid

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**SiF$_6^{2-}$**

Lewis Structure:

Areas of charge density: 6

Geometry: Octahedral
Bonding Based on Linear Geometry

Bonding Based on Trigonal Planar Geometry

Bonding Based on Tetrahedral Geometry
9.2 Given a molecule, draw its Lewis Structure and predict the polarity of the molecule. [Readings 9.3 Problems 6-9, 62, & 63]
Polar Bonds and Polar Molecules

The arrangement of polar bonds around the central atom determines if the molecule is polar.
The molecule is not polar if:
- the bonded atoms are arranged symmetrically,
- and the bonded atoms are the same or have the same electronegativities.
(i.e. the vector sum of the polar bonds is zero.)
Otherwise the molecule is polar.
The partial charge distribution is the vector sum of the polar bonds.

Examples:
- $\text{CO}_2$
- $\text{H}_2\text{O}$
- $\text{H}_2\text{CO}$
Polar Bonds and Polar Molecules
Examples:

CO₂

H₂O

H₂CO

Polarity of molecules affect their properties.
Polar Bonds and Polar Molecules

- Water is a polar molecule

9.3 Predict the types of orbitals (including hybrids) involved in bonding and resulting bond types (sigma, pi). [Readings 9.4 - 9.5 Problems 29, 31, 80, 81, & 84]

Atomic Orbitals and Bonding

$F_2$

\[ \text{↑} \quad \text{↓} \quad \text{↑} \quad \text{↓} \quad \text{↑} \]

\[ \text{↓} \quad \text{↑} \quad \text{↓} \text{↑} \text{↓} \text{↑} \text{↓} \text{↓} \]

\[ \text{↓} \quad \text{↑} \quad \text{↓} \text{↑} \text{↓} \text{↑} \text{↓} \text{↓} \]

\[ \text{↓} \quad \text{↑} \quad \text{↓} \text{↑} \text{↓} \text{↑} \text{↓} \text{↓} \]
Atomic Orbitals and Bonding
\[ \text{O}_2 \]

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

\[ \text{\begin{tabular}{c}
  s\text{O} & 1s^22s^22p_x2p_y2p_z \\
  s\text{O} & 1s^22s^22p_x2p_y2p_z
\end{tabular}} \]

\[ \begin{array}{c}
  \uparrow \downarrow \uparrow \\
  \downarrow \uparrow \downarrow
\end{array} \]

\[ \begin{array}{c}
  \text{Sigma (\sigma) Bond} \\
  \text{Pi (\pi) Bond}
\end{array} \]
Hybrid Orbitals

\[ \text{CH}_4 - \text{Methane} \]

\[ \begin{array}{c}
\text{C} & 1s^22s^22p^2 \\
\uparrow & \uparrow & \uparrow \\
\hline
\text{H} & 1s^1 \\
\downarrow \\
\text{H} & 1s^1 \\
\downarrow \\
\text{H} & 1s^1 \\
\end{array} \]

Two bonds?

Promotion

Gain more in bonding than is lost in promotion.

\[ \text{CH}_4 - \text{Methane} \]

\[ \begin{array}{c}
\text{C} & 1s^22s^22p^2 \\
\uparrow & \uparrow \\
\hline
\text{H} & 1s^1 \\
\end{array} \]
Evidence shows these bonds are equivalent.
Mix the one 2s orbital with the three 2p orbitals to make four sp\(^3\) hybrid orbitals.
Hybrid Orbitals
Mix the one 2s orbital with the three 2p orbitals to make four sp^3 hybrid orbitals.

These hybrids explain the geometries of molecules.
Mix the one 2s orbital with the three 2p orbitals to make four sp^3 hybrid orbitals.

These hybrids explain the geometries of molecules.

Hybrid Orbital Types

<table>
<thead>
<tr>
<th># electron pairs</th>
<th>AO</th>
<th>Hybrid orbitals</th>
<th>Orientation</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>s,p</td>
<td>sp</td>
<td>linear</td>
<td>BeF_2</td>
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<td>2</td>
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<td>BeF₂</td>
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<tr>
<td>3</td>
<td>s,p,p</td>
<td>sp²</td>
<td>trigonal planar</td>
<td>BF₃</td>
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<tr>
<td>4</td>
<td>s,p,p,p</td>
<td>sp³</td>
<td>tetrahedral</td>
<td>CH₄</td>
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<tr>
<td>5</td>
<td>s,p,p,d,d</td>
<td>dsp³</td>
<td>trigonal bipyramid</td>
<td>PCl₅</td>
</tr>
<tr>
<td>6</td>
<td>s,p,p,d,d,d</td>
<td>d²sp³</td>
<td>octahedral</td>
<td>SF₆</td>
</tr>
</tbody>
</table>
Each carbon has three \( sp^2 \) hybrid orbitals and one \( p \) orbital.

3 areas of electron density

\( sp^2 \) hybrid orbitals needed