Worksheet 15 - Molecular Shapes

The shapes of molecules can be predicted from their Lewis structures by using the VSEPR (Valence Shell Electron Pair Repulsion) model, which states that electron pairs around a central atom will assume a geometry that keeps them as far apart from each other as possible.

This is illustrated by the drawings below.

Six groups surrounding a central atom will form an octahedron. All of the groups in this structure are at $90^\circ$ or $180^\circ$ to each other. All positions are equivalent.

Five groups will form a trigonal bipyramid. The two positions pointing up and down are called the axial positions. They are at $180^\circ$ to each other, and at $90^\circ$ to the other three, equatorial positions. The three equatorial positions are at $120^\circ$ to each other. There is more room in the equatorial positions, and large groups will occupy these positions.

Four groups will form a tetrahedron. All of the angles in a tetrahedron are $109.5^\circ$, and all positions are equivalent.

Three groups will form a flat triangle (trigonal planar). Each of the angles is $120^\circ$ and all positions are equivalent.

Two groups form a straight line (linear) with $180^\circ$ between them.

How does this apply to Chemistry?

The groups occupying these geometric positions will be either atoms bonded to the central atom, or lone pair electrons on the central atom.

Lone pair electrons occupy more space than bonded electrons, so they will take the equatorial position in the trigonal bipyramid.

Lone pair electrons will also occupy positions that put them as far apart from each other as possible.
1. Draw the Lewis structure for water, H₂O.

   \[
   \text{H:O:H}
   \]

   \[
   \text{\( \delta^+ \rightarrow O \rightarrow \delta^- \)}
   \]

   \[
   \text{\( \rightarrow \)}
   \]

   a) How many "groups" (atoms and lone pairs) surround the central oxygen? 
      2 atoms + 2 lone pairs

   b) What is the geometry of this molecule (look at atoms and lone pairs)? Draw this VSEPR structure next to the Lewis structure.
      \[\text{tetrahedral}\]

   c) What is the shape of this molecule (look only at the atoms)?
      \[\text{bent}\]

   d) What is the H-O-H bond angle? \[\approx 109.5^\circ\]

   e) Place the partial positive and negative charges on the H and O atoms, based on their relative electronegativities. Is water a polar compound?
      \[\text{yes}\]

2. Draw the Lewis structure for NO₂⁻. \[5 + 2 + 1 = 8 e^-\]

   \[
   \text{\'O'-N-O'\')}
   \]

   \[
   \text{\( \delta^+ \rightarrow N \rightarrow \delta^- \)}
   \]

   a) How many "groups" (atoms and lone pairs) surround the central nitrogen? 
      2 bonding pairs + 1 lone pair (ignore =)

   b) What is the geometry of this molecule (look at atoms and lone pairs)? Draw this VSEPR structure next to the Lewis structure.
      \[\text{trigonal planar}\]

   c) What is the shape of this molecule (look only at the atoms)?
      \[\text{bent}\]

   d) What is the O-N-O bond angle? \[\approx 120^\circ\]

   e) Place the partial positive and negative charges on the N and O atoms, based on their relative electronegativities. Is NO₂⁻ a polar compound?
      \[\text{it is polar}\]
3. Draw the Lewis and VSEPR structures for the following 12 compounds and label them with their geometry.

<table>
<thead>
<tr>
<th>Lewis</th>
<th>VSEPR</th>
<th>Lewis</th>
<th>VSEPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) SF₆</td>
<td>6+12=18e⁻</td>
<td>6</td>
<td>( \text{VSEPR: octahedral} )</td>
</tr>
<tr>
<td>( \text{Octahedral} )</td>
<td></td>
<td></td>
<td>( \text{Octahedral} )</td>
</tr>
<tr>
<td>c) ICl₄⁻</td>
<td>7+28+1=36e⁻</td>
<td>4</td>
<td>( \text{VSEPR: octahedral} )</td>
</tr>
<tr>
<td>( \text{Tetrahedral} )</td>
<td></td>
<td></td>
<td>( \text{Tetrahedral} )</td>
</tr>
<tr>
<td>e) CF₄</td>
<td>4+16=20e⁻</td>
<td>4</td>
<td>( \text{VSEPR: tetrahedral} )</td>
</tr>
<tr>
<td>( \text{Tetrahedral} )</td>
<td></td>
<td></td>
<td>( \text{Tetrahedral} )</td>
</tr>
<tr>
<td>g) BrF₃</td>
<td>7+21=28e⁻</td>
<td>3</td>
<td>( \text{VSEPR: trigonal bipyramidal} )</td>
</tr>
<tr>
<td>( \text{Trigonal Bipyramidal} )</td>
<td></td>
<td></td>
<td>( \text{Tetrahedral} )</td>
</tr>
<tr>
<td>i) CO₂</td>
<td>2+12=14e⁻</td>
<td>2</td>
<td>( \text{VSEPR: linear} )</td>
</tr>
<tr>
<td>( \text{Linear} )</td>
<td></td>
<td></td>
<td>( \text{Octahedral} )</td>
</tr>
<tr>
<td>k) SO₃</td>
<td>6+18=24e⁻</td>
<td>3</td>
<td>( \text{VSEPR: trigonal planar} )</td>
</tr>
<tr>
<td>( \text{Trigonal Planar} )</td>
<td></td>
<td></td>
<td>( \text{Trigonal Bipyramidal} )</td>
</tr>
</tbody>
</table>
Now fill in the missing information in the chart using the structures you have drawn in problems 1 - 3.

<table>
<thead>
<tr>
<th>compound</th>
<th>atoms on central atom</th>
<th>lone pairs on central atom</th>
<th>geometry</th>
<th>shape</th>
<th>polar</th>
</tr>
</thead>
<tbody>
<tr>
<td>SF₆</td>
<td>6</td>
<td>0</td>
<td>octahedral</td>
<td>octahedral</td>
<td>no</td>
</tr>
<tr>
<td>BrF₅</td>
<td>5</td>
<td>1</td>
<td>octahedral</td>
<td>square pyramidal</td>
<td>yes</td>
</tr>
<tr>
<td>I₄⁻</td>
<td>4</td>
<td>2</td>
<td>octahedral</td>
<td>square planar</td>
<td>no</td>
</tr>
<tr>
<td>XeCl₃⁻</td>
<td>3</td>
<td>3</td>
<td>octahedral</td>
<td>T</td>
<td>yes</td>
</tr>
<tr>
<td>PF₅</td>
<td>5</td>
<td>0</td>
<td>bipyramidal</td>
<td>bipyramidal</td>
<td>no</td>
</tr>
<tr>
<td>SF₄</td>
<td>4</td>
<td>1</td>
<td>bipyramidal</td>
<td>seesaw</td>
<td>yes</td>
</tr>
<tr>
<td>BrF₃</td>
<td>3</td>
<td>2</td>
<td>bipyramidal</td>
<td>T</td>
<td>yes</td>
</tr>
<tr>
<td>I₅⁻</td>
<td>2</td>
<td>3</td>
<td>trigonal bipyramidal</td>
<td>linear</td>
<td>no</td>
</tr>
<tr>
<td>CF₄</td>
<td>4</td>
<td>0</td>
<td>tetrahedral</td>
<td>tetrahedral</td>
<td>no</td>
</tr>
<tr>
<td>NH₃</td>
<td>3</td>
<td>1</td>
<td>tetrahedral</td>
<td>trigonal pyramidal</td>
<td>yes</td>
</tr>
<tr>
<td>H₂O</td>
<td>2</td>
<td>2</td>
<td>tetrahedral</td>
<td>V-shaped (bent)</td>
<td>yes</td>
</tr>
<tr>
<td>SO₃</td>
<td>3</td>
<td>0</td>
<td>trigonal planar</td>
<td>trigonal planar</td>
<td>no</td>
</tr>
<tr>
<td>NO₂⁻</td>
<td>2</td>
<td>1</td>
<td>trigonal planar</td>
<td>bent</td>
<td>yes</td>
</tr>
<tr>
<td>CO₂</td>
<td>2</td>
<td>0</td>
<td>linear</td>
<td>linear</td>
<td>no</td>
</tr>
</tbody>
</table>