The 3D Shape of a molecule can be predicted using *Valence Shell Electron Pair Repulsion (VSEPR)* theory.

Basic idea: Because of repulsion between electrons, molecules will adopt a shape that allows the electrons in bonds and lone pairs to be located as far as possible from each other.

The shape of a molecule depends on the number of **electron groups** around the central atom.

- Electron groups are other atoms bonded to the central atom, or lone pairs on the central atom.
Two Electron Groups: Linear Geometry
Three Electron Groups: Trigonal Planar Geometry

Trigonal planar geometry

- B (boron) bonded with three fluorine (F) atoms, forming an angle of 120°.

- C (carbon) bonded with two hydrogen (H) and one oxygen (O) atoms, forming angles of 121.9° and 116.2°.
Four Electron Groups: Tetrahedral Geometry
10.3 VSEPR: The Effect of Lone Pairs

- Ozone has three electron groups around the central oxygen, so has the **trigonal planar electron geometry**.
- The **molecular geometry** is bent:
The Effect of Lone Pairs (contd.)

- With four electron groups (tetrahedral electron geometry), there can be one or two lone pairs around the central atom.
- Lone pairs repel more than bonds, so increasing the number of lone pairs decreases the bond angles.
Figure 10.4 Effect of Lone Pairs on Molecular Geometry

- **No lone pairs**
  - CH$_4$
  - 109.5°

- **One lone pair**
  - NH$_3$
  - 107°

- **Two lone pairs**
  - H$_2$O
  - 104.5°
Five Electron Groups: Trigonal Bipyramidal Geometry
Trigonal Bipyramidal Geometry (contd.)

Lone pairs are **always equatorial** to minimize $90^\circ$ interactions.

![Diagram showing molecular geometries and bond angles](image-url)
Six Electron Groups: Octahedral Geometry
Octahedral Geometry (contd.)

One lone pair:

Two lone pairs:
Lone pairs are 180° from each other
10.4: VSEPR Theory: Predicting Molecular Geometries

To determine the shape of a molecule, follow these steps:

1. Draw the molecule’s Lewis structure.
2. Determine the total number of electron groups around the central atom.
3. The number of electron groups (2, 3, 4, 5 or 6) determines the “electron geometry,” the basic shape and ideal angles.
4. If there are lone pair(s) on the central atom, the shape will be one of the variations of the basic geometries (“molecular geometry”).
<table>
<thead>
<tr>
<th>Electron Groups*</th>
<th>Bonding Groups</th>
<th>Lone Pairs</th>
<th>Electron Geometry</th>
<th>Molecular Geometry</th>
<th>Approximate Bond Angles</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>Linear</td>
<td>Linear</td>
<td>180°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>0</td>
<td>Trigonal planar</td>
<td>Trigonal planar</td>
<td>120°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>1</td>
<td>Trigonal planar</td>
<td>Bent</td>
<td>&lt;120°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>0</td>
<td>Tetrahedral</td>
<td>Tetrahedral</td>
<td>109.5°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>1</td>
<td>Tetrahedral</td>
<td>Trigonal pyramidal</td>
<td>&lt;109.5°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>2</td>
<td>Tetrahedral</td>
<td>Bent</td>
<td>&lt;109.5°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>5</td>
<td>5</td>
<td>0</td>
<td>Trigonal bipyramidal</td>
<td>Trigonal bipyramidal</td>
<td>120° (equatorial) 90° (axial)</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>1</td>
<td>Trigonal bipyramidal</td>
<td>Seesaw</td>
<td>&lt;120° (equatorial) &lt;90° (axial)</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>2</td>
<td>Trigonal bipyramidal</td>
<td>T-shaped</td>
<td>&lt;90°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>3</td>
<td>Trigonal bipyramidal</td>
<td>Linear</td>
<td>180°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>0</td>
<td>Octahedral</td>
<td>Octahedral</td>
<td>90°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>6</td>
<td>5</td>
<td>1</td>
<td>Octahedral</td>
<td>Square pyramidal</td>
<td>&lt;90°</td>
<td><img src="image" alt="Example" /></td>
</tr>
<tr>
<td>6</td>
<td>4</td>
<td>2</td>
<td>Octahedral</td>
<td>Square planar</td>
<td>90°</td>
<td><img src="image" alt="Example" /></td>
</tr>
</tbody>
</table>

*Count only electron groups around the central atom. Each of the following is considered one electron group: a lone pair, a single bond, a double bond, a triple bond, or a single electron.

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Wedge-Dash Notation

- A way to represent 3D molecular structures on paper (p. 437):
Molecules With More Than One Central Atom

Consider the geometry of each atom separately.
- See the example of glycine, p. 437.
10.5: Molecular Shape and Polarity

- Polar bonds have **dipole moments**:

  ![Polar bond](image)

  ![Net dipole moment](image)

  ![Low electron density](image)

  ![High electron density](image)
Molecular Shape and Polarity (contd.)

- For molecules with more than one bond, if the dipole moments combine to give a net dipole, the molecule is polar.
- In CO$_2$, the dipoles of the bonds cancel.
- So it is a **nonpolar molecule that has polar bonds**.
Molecular Shape and Polarity (contd.)

• In contrast, because water has a bent geometry the dipole moments combine to give a net dipole, so it is polar.
Molecular Shape and Polarity (contd.)

<table>
<thead>
<tr>
<th>TABLE 10.2 Common Cases of Adding Dipole Moments to Determine whether a Molecule Is Polar</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Linear</strong></td>
</tr>
<tr>
<td>Nonpolar</td>
</tr>
<tr>
<td>The dipole moments of two identical polar bonds pointing in opposite directions will cancel. The molecule is nonpolar.</td>
</tr>
<tr>
<td><strong>Trigonal planar</strong></td>
</tr>
<tr>
<td>Nonpolar</td>
</tr>
<tr>
<td>The dipole moments of three identical polar bonds at 120° from each other will cancel. The molecule is nonpolar.</td>
</tr>
<tr>
<td><strong>Trigonal pyramidal</strong></td>
</tr>
<tr>
<td>Polar</td>
</tr>
<tr>
<td>The dipole moments of three polar bonds in a trigonal pyramidal arrangement (109.5° from each other) will not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.</td>
</tr>
</tbody>
</table>

Note: In all cases where the dipoles of two or more polar bonds cancel, the bonds are assumed to be identical. If one or more of the bonds are different from the other(s), the dipoles will not cancel and the molecule will be polar.