VSEPR Theory

- In any molecule or ion there are regions of high electron density:
  - Bonds (shared electron pairs)
  - Lone pairs (unshared electrons)
- Due to electron-electron repulsion, these regions are arranged as far apart as possible
- Such arrangement results in the minimum energy for the system
Five Basic Geometries

- Linear
- Trigonal
- Trigonal bipyramidal
- Tetrahedral
- Octahedral
CH$_4$, NH$_3$, and H$_2$O

- These molecules have the same electronic geometry but different molecular geometry
Electronic Geometry and Molecular Geometry

- **Electronic geometry**
  - Distribution of regions of high electron density around the central atom

- **Molecular geometry**
  - Arrangement of atoms around the central atom

- If a molecule does not have lone electron pairs, both geometries are the same

- If lone pairs are present, molecular and electronic geometries are different
BeH$_2$ and H$_2$O
Polar and Nonpolar Molecules

- **Nonpolar Molecule**
  - Dipole moments for all bonds cancel out

- **Polar Molecule**
  - Dipole moments for all bonds don’t cancel out – the molecule has the resulting net dipole moment
$\text{BBr}_3$ and $\text{SO}_2$
Bond angles in CH$_4$, NH$_3$, H$_2$O

- VSEPR theory:
  - A lone pair takes up more space than a bond
Polarity of CH$_4$, NH$_3$, H$_2$O

- Red - more electron density (more negative)
- Blue - less electron density (more positive)
Bond angles in NH₃ and NF₃

- More electronegative atoms pull electron density away from the central atom
- The region around the central atom becomes less crowded and the bond angles decrease

NH₃: 107.3°  
NF₃: 102.1°
$PF_5$, $SF_4$, $ClF_3$, and $XeF_2$
$\text{PF}_5, \text{SF}_4, \text{ClF}_3, \text{and XeF}_2$
The Lone Pair in SF₄

- There are 2 different positions in the trigonal bipyramid: axial and equatorial.
- Where does the lone pair go first?

3 bonds at 90°
1 bond at 180°

2 bonds at 90°
2 bonds at 120°
$\text{SF}_4$: Seesaw Shape
**ClF₃ and XeF₂**

- In these molecules the 2nd and 3rd lone pairs still prefer to occupy the equatorial sites.
- In this way, the lone pairs are arranged farther apart from each other.

![ClF₃ T-shaped](image1)

![XeF₂ Linear](image2)
TBP Electronic Geometry

- If lone pairs are incorporated into the trigonal bipyramidal structure, they occupy equatorial positions.

  - There are 3 possible shapes:
    - 1 lone pair - Seesaw shape
    - 2 lone pairs - T-shape
    - 3 lone pairs - Linear
$\text{SeF}_6$, $\text{IF}_5$, and $\text{XeF}_4$
SeF$_6$: Octahedron

All bond angles are 90°
IF$_5$ and XeF$_4$

- The 1st lone pair can occupy any site
- The 2nd lone pair is arranged opposite to the 1st
Octahedral Electronic Geometry

- If lone pairs are incorporated into the octahedral structure, there are 2 possible new shapes
  - 1 lone pair - Square pyramid
  - 2 lone pairs - Square planar
Assignments & Reminders

- Go through the lecture notes
- Read Chapter 8 completely
- Homework #5 covers Chapters 7 & 8 and is due by Oct. 31
- Monday (10/24) and Tuesday (10/25) – lab quiz #2 (Experiments A, #5 & #9)