Molecular Geometry (Shapes) – VSEPR Theory

VSEPR – Valence Shell Electron Pair Repulsion theory – electron pairs repel each other, thus will electron pairs will be found as far apart from each other as possible.

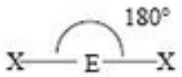
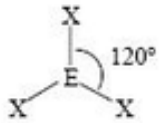
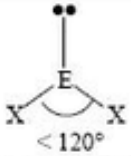
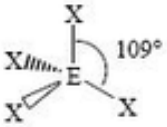
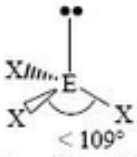
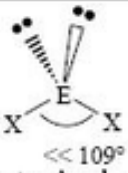
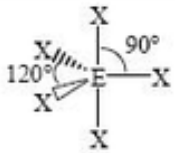
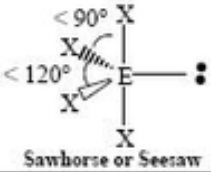
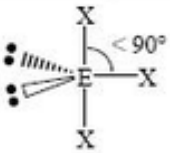
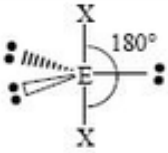
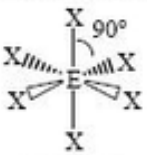
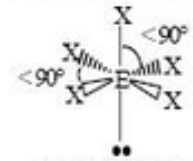
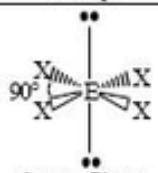
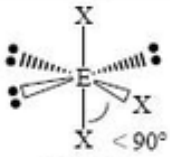
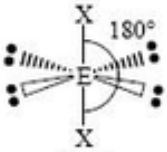
Steps for Determining Molecular Geometry (shape)

1. Draw the Lewis structure.
2. Count the number of electron domains around the central atom.
    a. Lone pair = one domain
    b. Any (single/double/triple) bond = one domain
3. The number of electron domains determines electron-domain geometry (basic geometry).
4. Determine the number of lone pairs.
5. The number of lone pairs determines molecular geometry (shape of the molecule).

Bond Angles

- Lone pairs have more repulsive forces compared to bonding pairs since they are closer to the central atom.
- Each lone pair around the central atom decreases the bond angle by approximately 2.5 degrees.

VSEPR Geometries

Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal Planar	 Bent or Angular			
4	 Tetrahedral	 Trigonal Pyramid	 Bent or Angular		
5	 Trigonal Bipyramid	 Sawhorse or Seesaw	 T-shape	 Linear	
6	 Octahedral	 Square Pyramid	 Square Planar	 T-shape	 Linear

Molecular Polarity

- NONPOLAR molecules have NO NET DIPOLE MOMENT, meaning an EQUAL distribution of electron density about the molecule.
- POLAR molecules have a NET DIPOLE MOMENT, meaning an UNEQUAL distribution of electron density about the molecule.
    - The unequal distribution of electron density creates a dipole moment – one side of the molecule has more electrons than the other
    - Polarity is indicated in two ways:
        1) "δ^+" on the positive end (or pole) and "δ^-" on the negative end (or pole)
        2) An arrow pointing toward the more electronegative atom indicating a shift of electrons toward that atom

Determining Molecular Polarity

- Determine the polarity of the bonds that make-up the molecule.
- If bond dipoles cancel each other, then the molecule is nonpolar.
- If bond dipoles do not cancel each other, resulting in a net dipole moment, then the molecule is polar.
- If lone pairs are present on the central atom the molecule is *typically* polar.
    - Lone pairs creates increased electron repulsion and thus, an unequal distribution of electron density, which repels the other electron regions (bonds) more.
    - Exceptions:
        - Trigonal bipyramidal structures that are linear are nonpolar.
        - Octahedral structures that are square planar are nonpolar.
- **When justifying polarity, write "there is an unequal distribution of charge on the molecule, thus the molecule has a net dipole moment".**