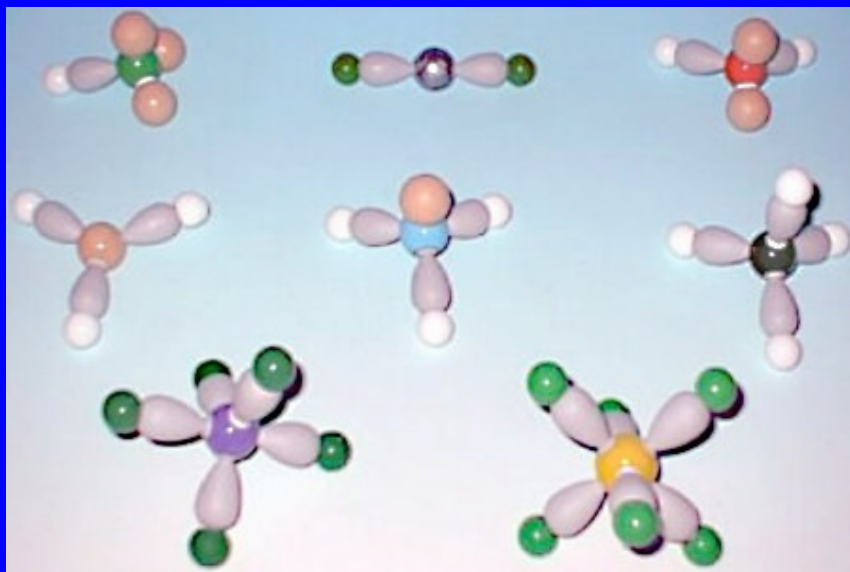
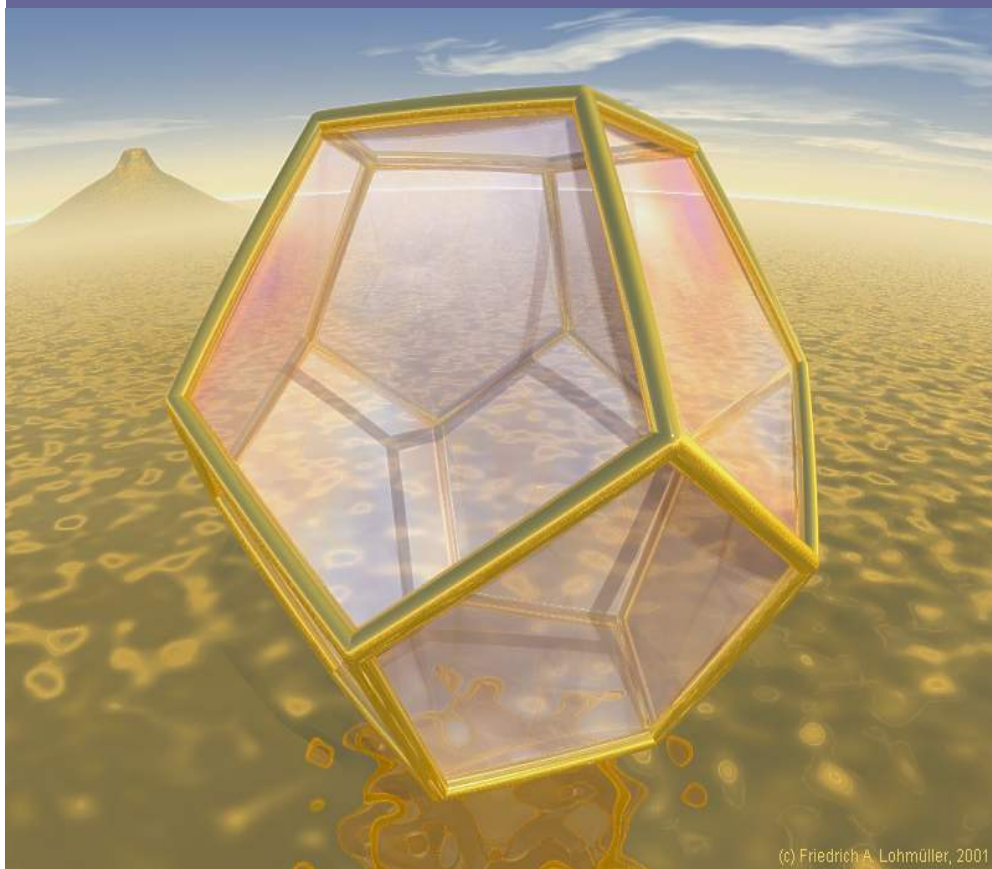


Section 6.5 – Molecular Geometry

- The properties of molecules depend on the bonding **and** the molecular geometry, the 3-dimensional arrangement of the atoms in space.



Molecular Geometry



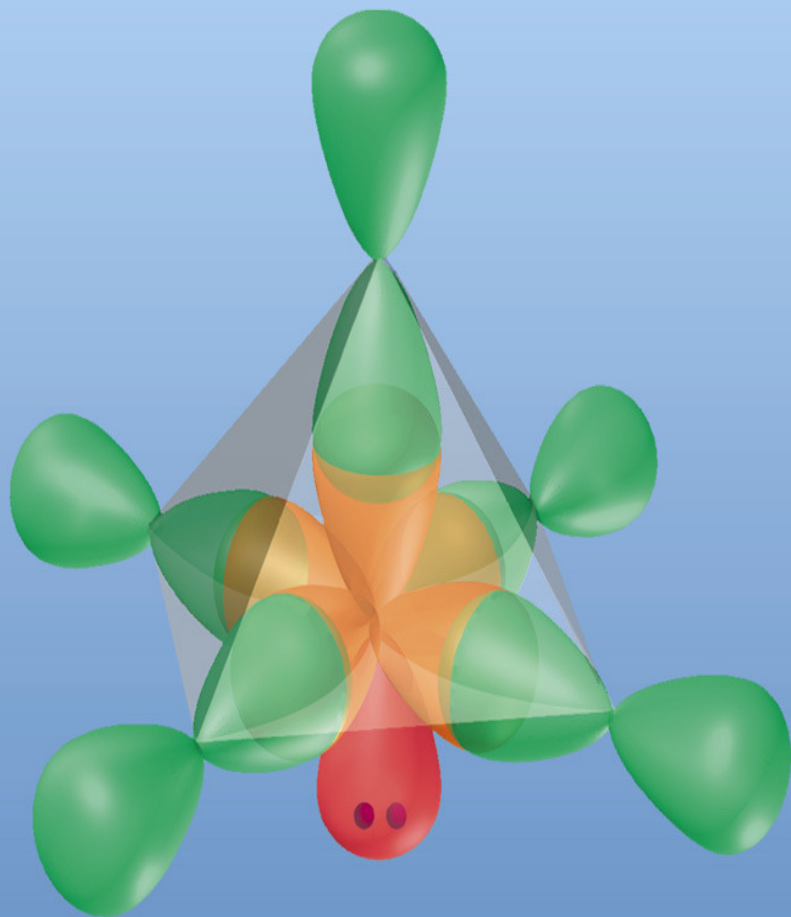
There are two different theories (VSEPR and hybridization) both based on experimental evidence, that can be used to describe this.

There Is No Conflict



- VSEPR Theory:
Accounts for molecular bond angles.
- Hybridization:
Describes the orbitals that contain the valence electrons of a molecule's atoms.

VSEPR Theory



Valence

Shell

Electron

Pair

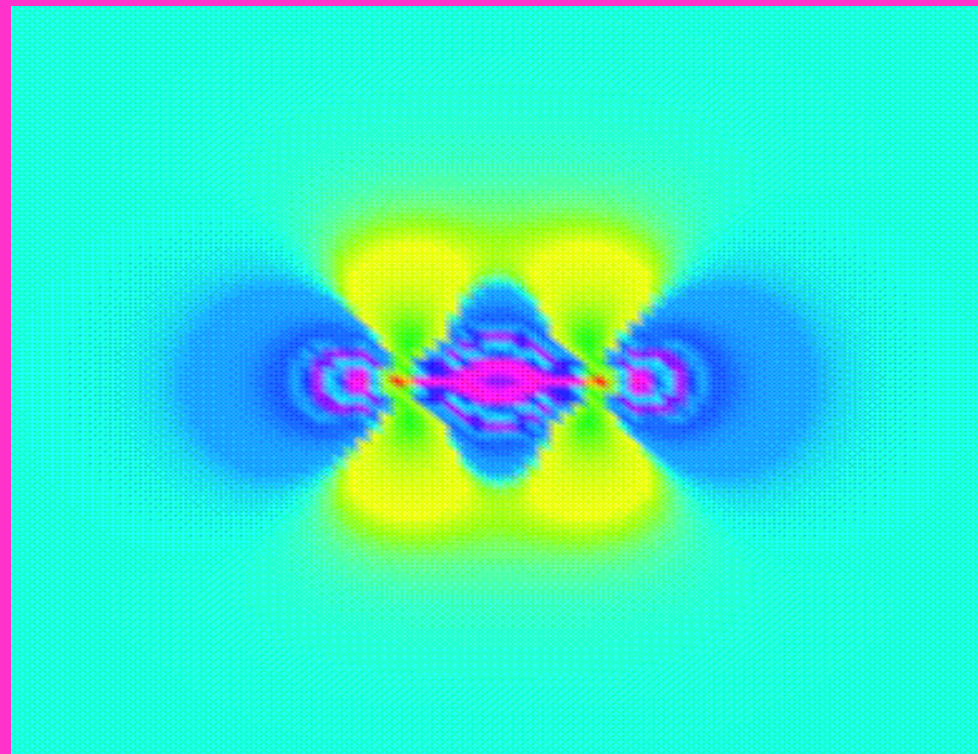
Repulsion

Repulsion between the valence-shell electrons surrounding an atom causes these sets to be oriented as far apart as possible.

Diatomic Molecules

- Diatomic molecules are composed of two atoms, so the geometry is *always* linear, with the molecular polarity being determined by the electronegativity differences between the atoms.

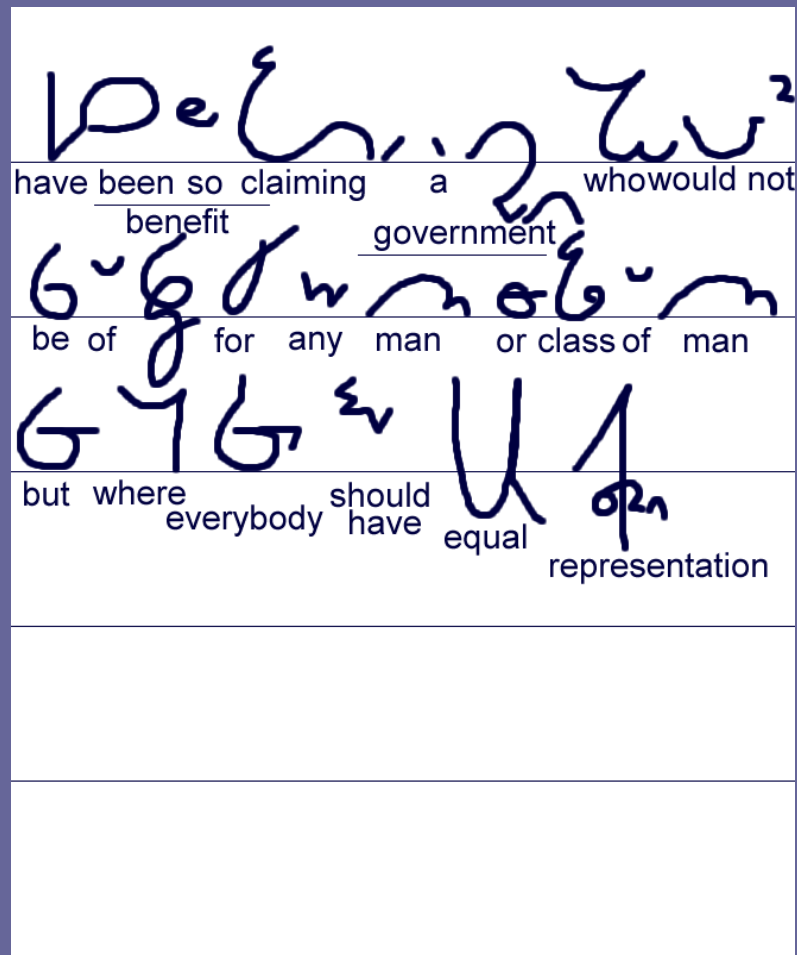
H₂: non-polar HCl: polar



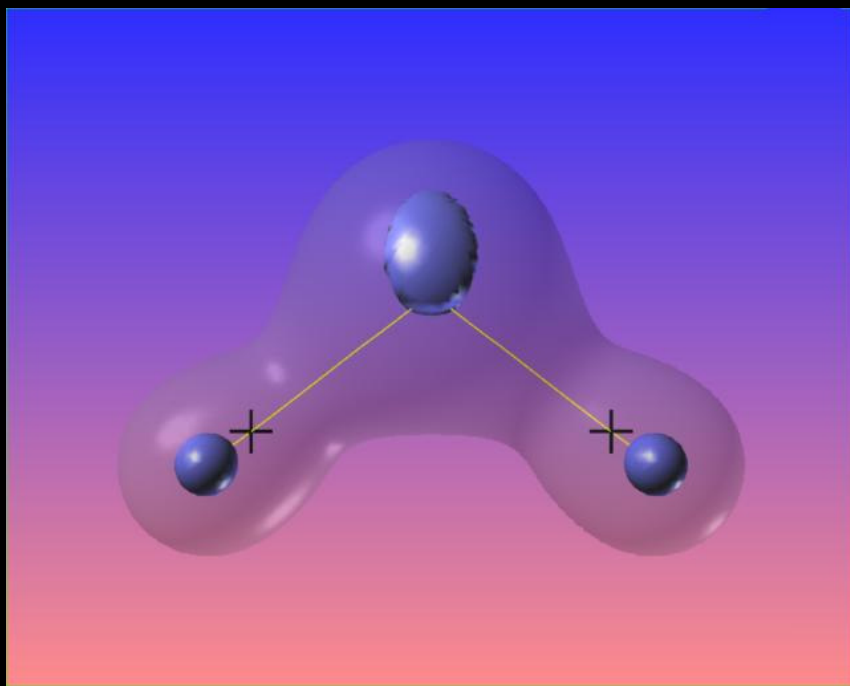
Electron distribution in N₂, triple bond in center of molecule, lone pairs on the outside of each N.

Shorthand for Describing

- For molecules containing more than two atoms, we can use the following symbols with subscripts:
 - A – the central atom
 - B – number of bonds on the central atom
 - E – number of lone pairs on central atom(for atoms that have multiple bonds, it is treated as a single B for geometry)



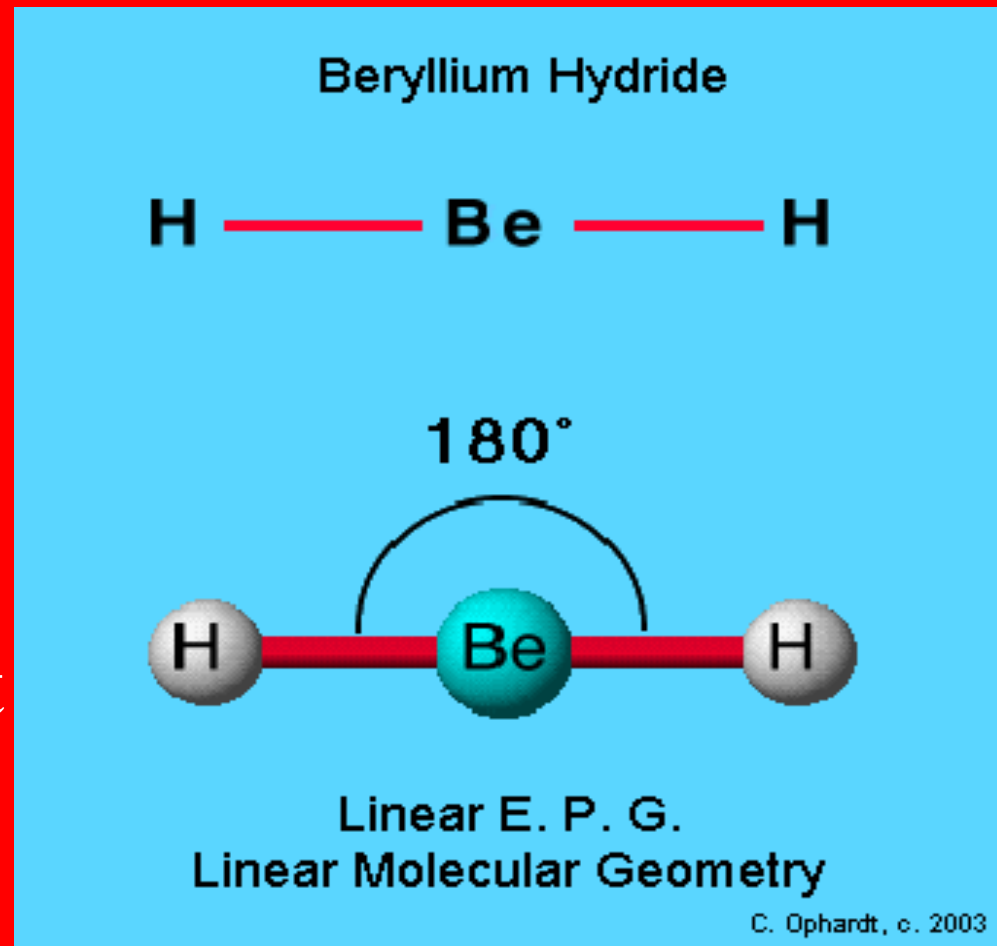
The Basis For VSEPR Theory



- That one must consider the locations of *all* electron pairs of the valence electrons in the molecule. Polyatomic ions are treated the same way. The following do *not* have lone pairs that influence the geometry of the molecule.

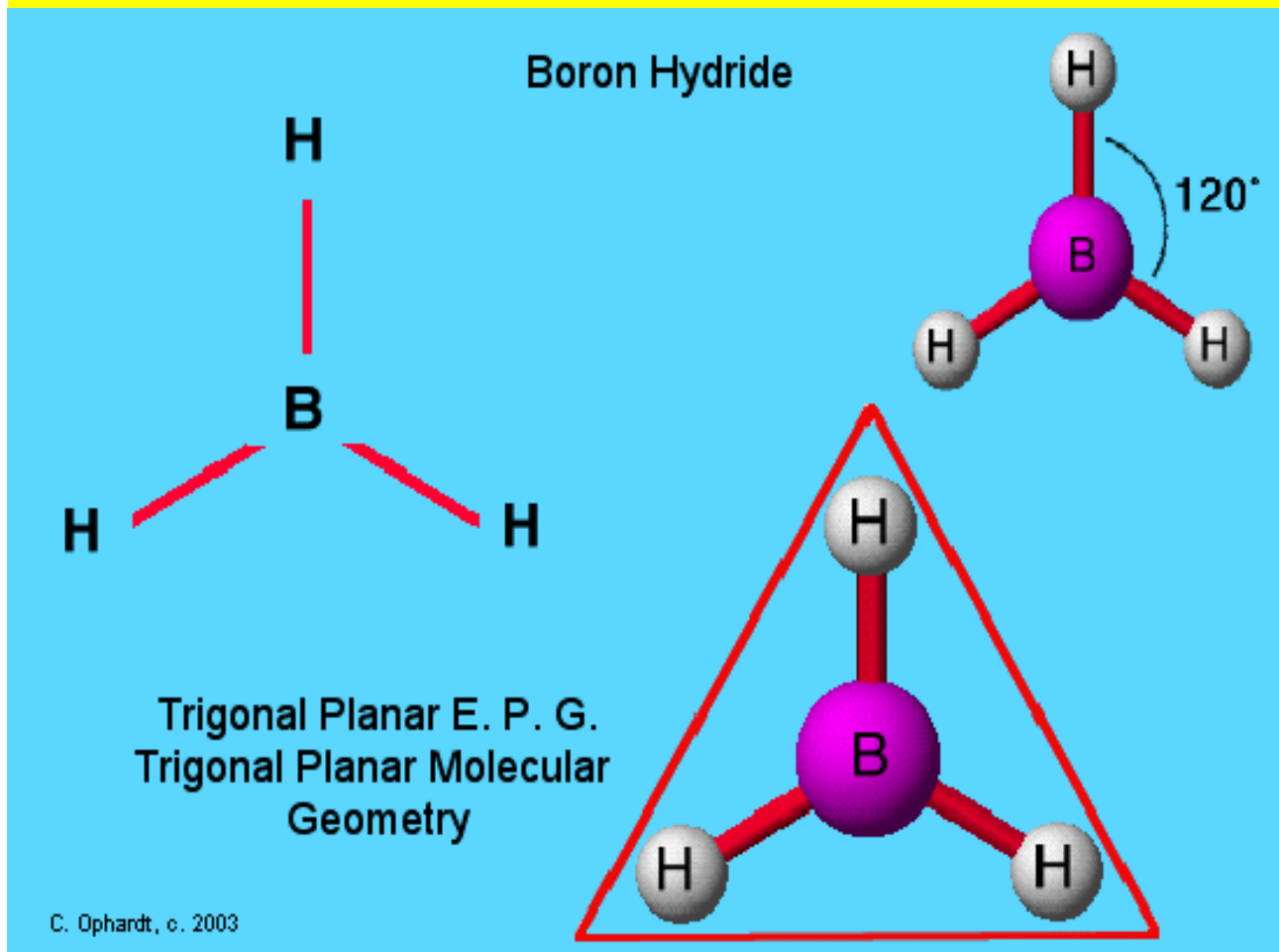
Linear – AB₂

- Central atom with two single bonds, no lone pairs. Because the valence electron pairs in the bonds repel each other, the bonds are as far apart as possible (180°).
- Ex: BeH₂



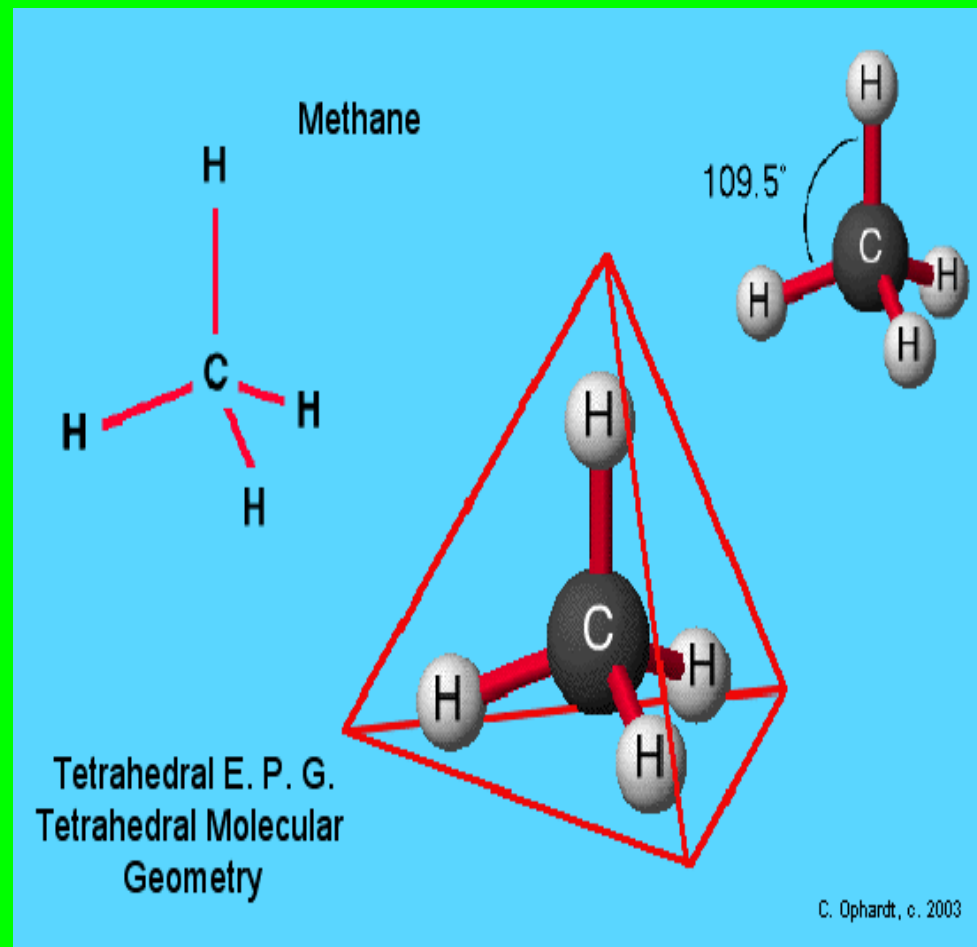
Trigonal Planar – AB₃

- The 3 A-B bonds stay furthest apart by pointing to the corners of an equilateral triangle, giving 120° angles between the bonds.



Tetrahedral – AB₄

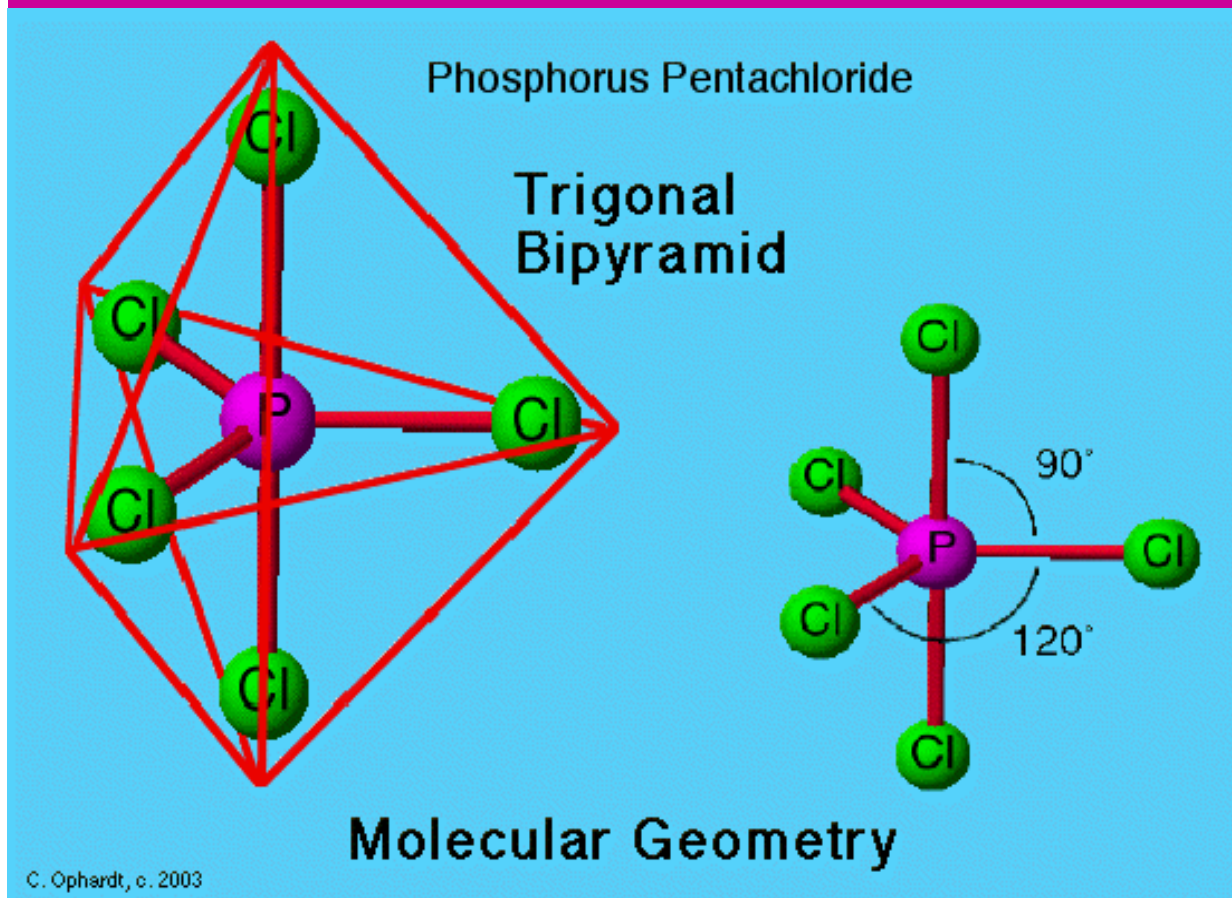
Octet rule is followed here. The distance between the A-B bonds is maximized if each bond points to the corners of a tetrahedron, giving bond angles of 109.5° between the bonds.



Ex.: CH₄

Trigonal-bipyramidal – AB₅

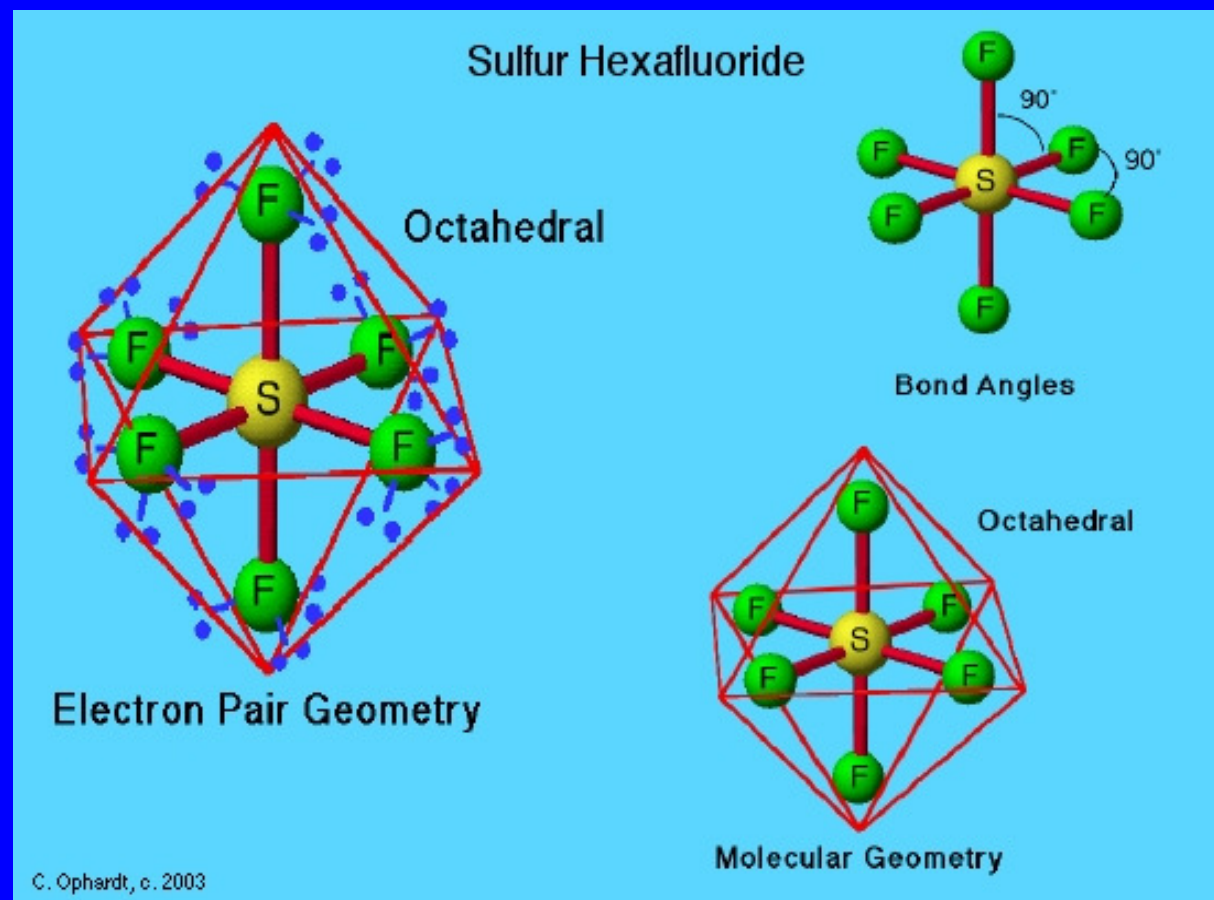
- 120° angles between bonds within the trigonal plane, 90° bond angles between the axial bond and those in the plane.



Ex.: PCl₅

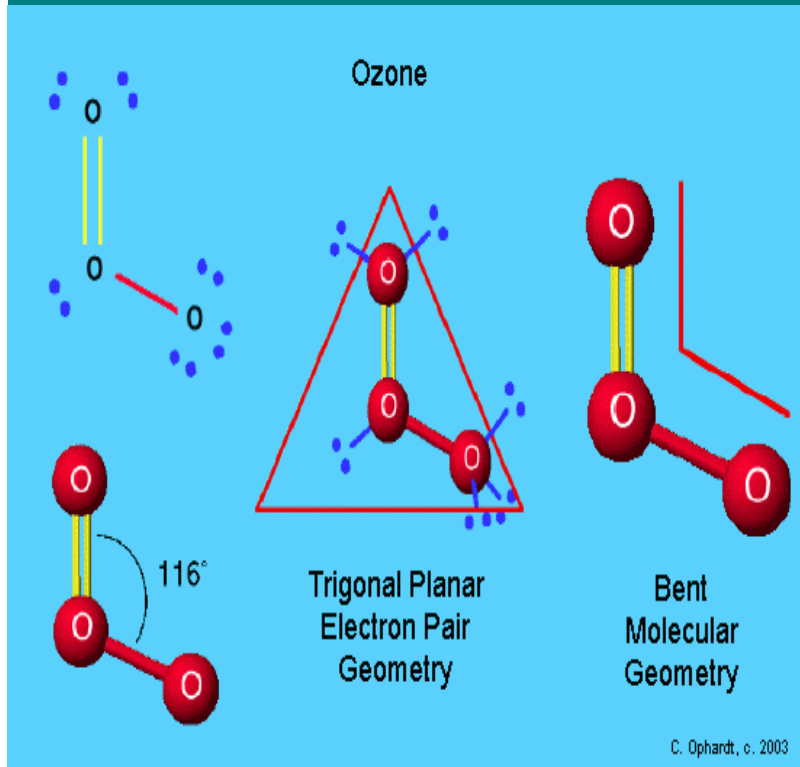
Octahedral – AB_6

6 bonds to the central atom, all equidistant from each other. 90° bond angles.



Ex.: SF_6

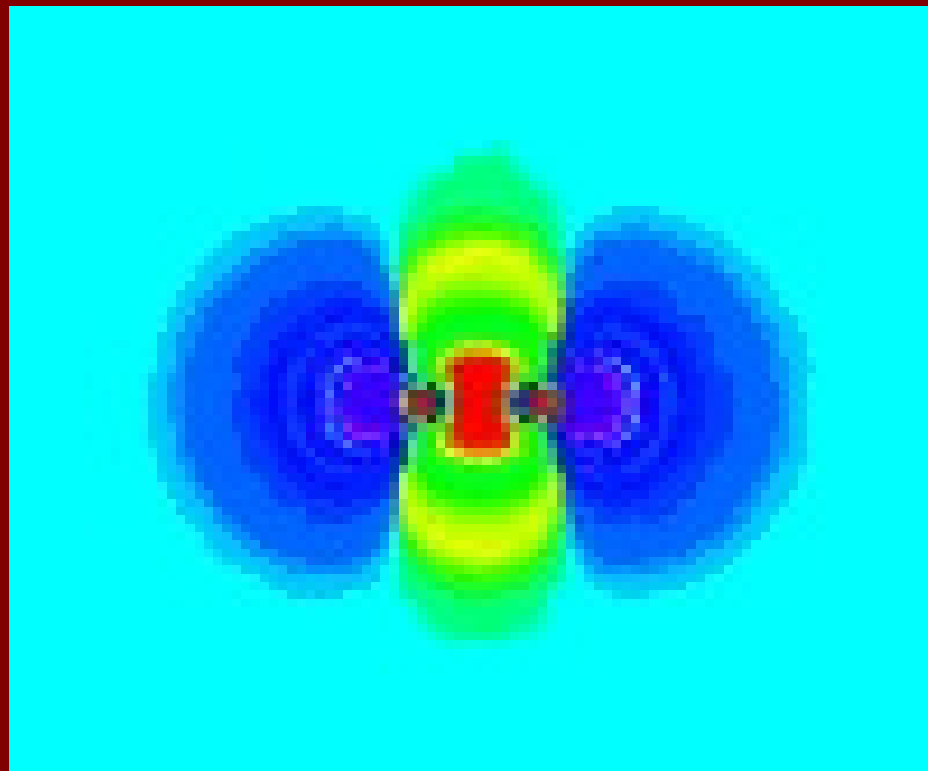
Lone Pairs Do Occupy Space and Influence Geometry



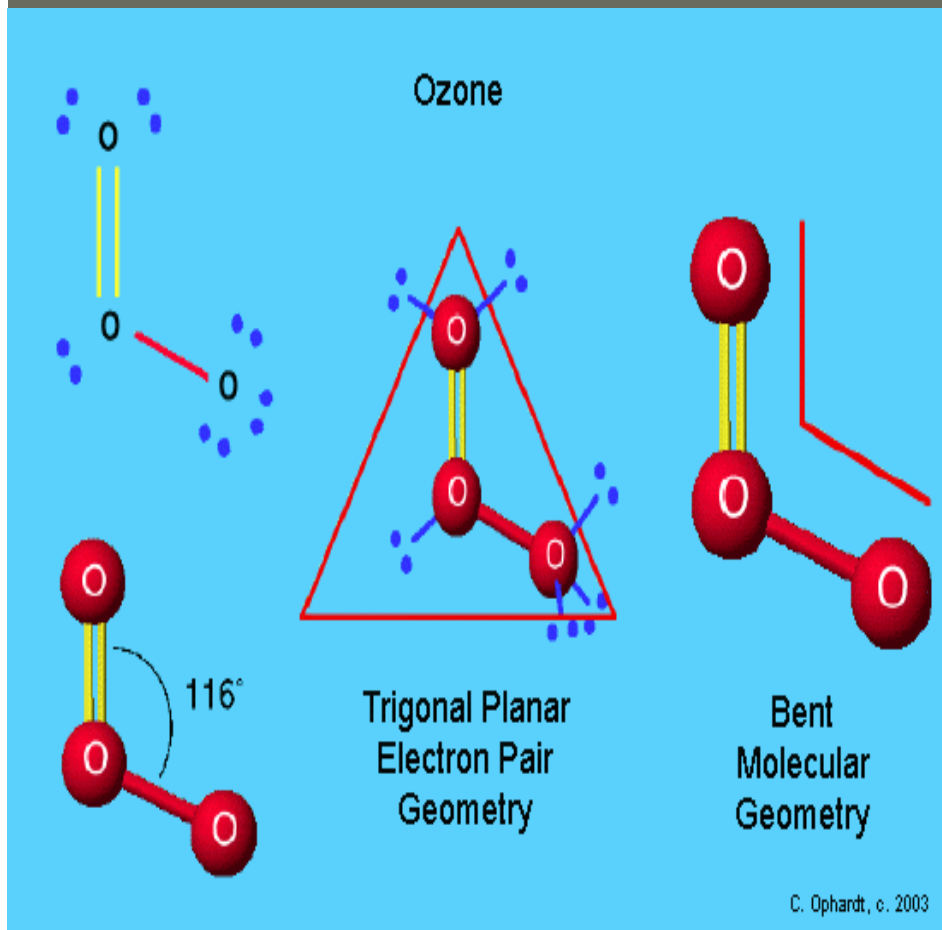
- But our description of the molecular geometry refers to the positions of the atoms *only*.
- Because lone pairs on central atoms are still electrons (regardless of whether they are being shared), they repel other electrons around the central atom

VSEPR and Unshared Electron Pairs

- One must always write out the Lewis structure for a molecule to decide on the proper geometry, the chemical formula of something does not tell you about lone pairs around the central atom.



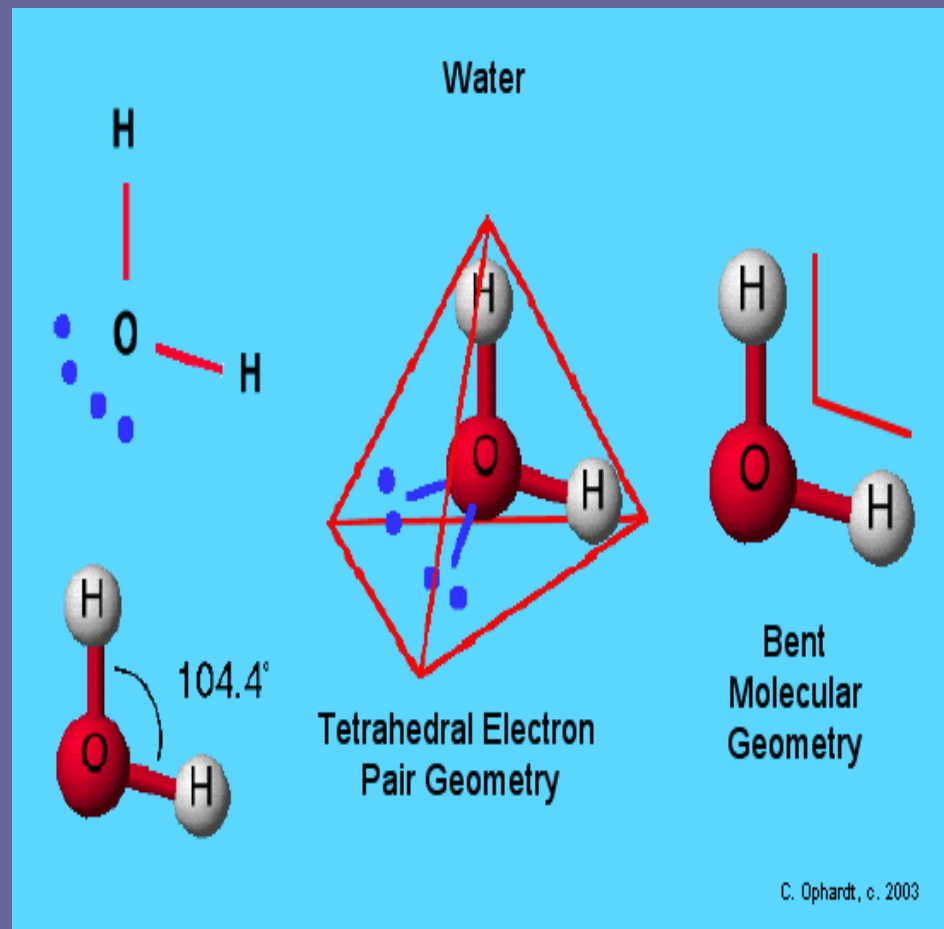
Bent – AB_2E



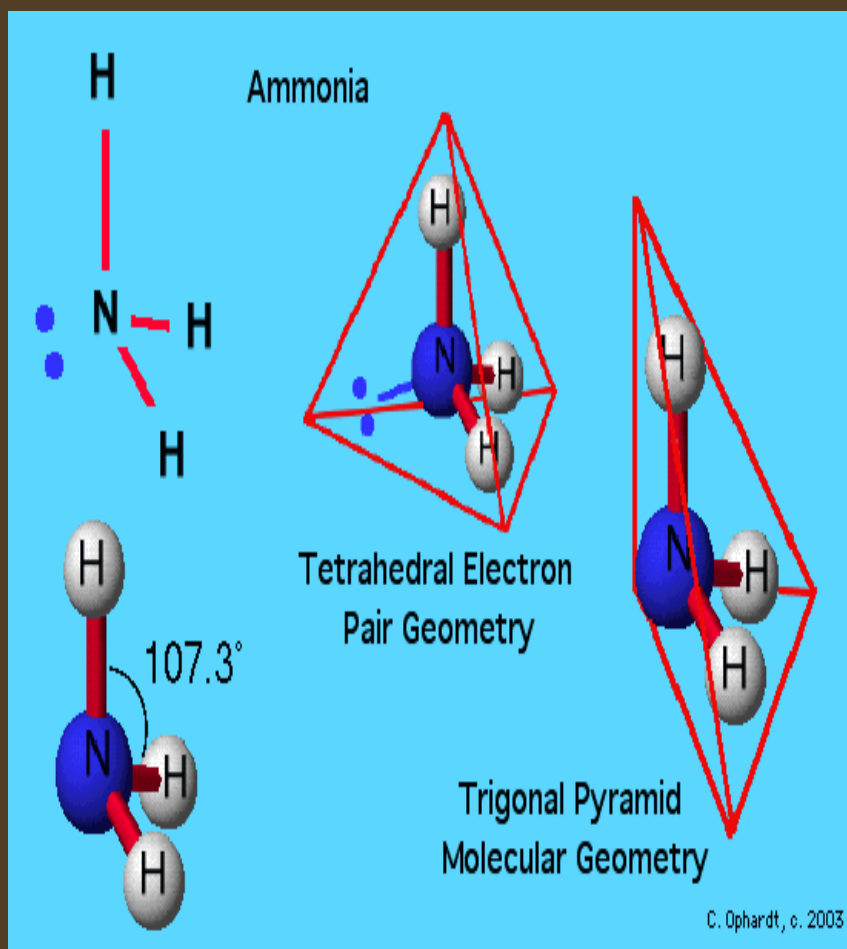
- 2 bonds to central atom with one lone pair. The lone pair bends what one would expect to be linear. The lone pair takes up more space than a bond and shoves the bonded atoms closer together than the 120° for trigonal planar.

Bent – AB_2E_2

- The addition of a second lone pair forces the bonding atoms even closer together than what one expects from tetrahedral.



Trigonal Pyramidal – AB_3E



- With 3 bonds one expects trigonal planar with 120° between the bonds, but the lone pair bends the plane away from the pair, forcing the atoms closer together.

Molecular Polarity

- Reflecting on the geometries, we can now see why lone pair on the central atom make a molecule polar—it changes the geometry of the molecule and creates an uneven electron “tug of war” across the molecule

