Tetrahedral Electronic Geometry: AB_3U Species (One Lone Pair of Electrons on A)

- Some examples of molecules with this geometry are:

  NH_3, NF_3, PH_3, PCl_3, AsH_3

- These molecules are our first examples of central atoms with lone pairs of electrons.

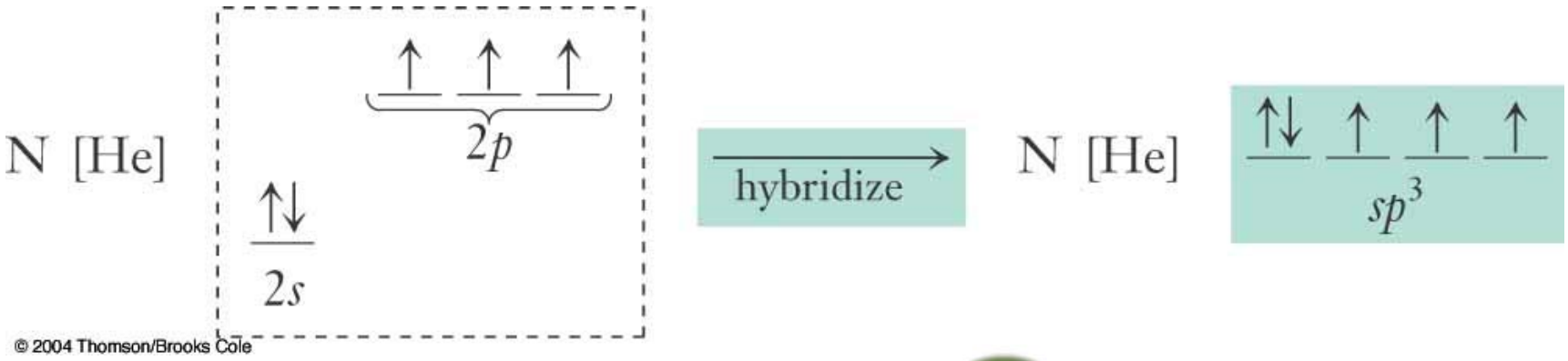
  Thus, the electronic and molecular geometries are different.

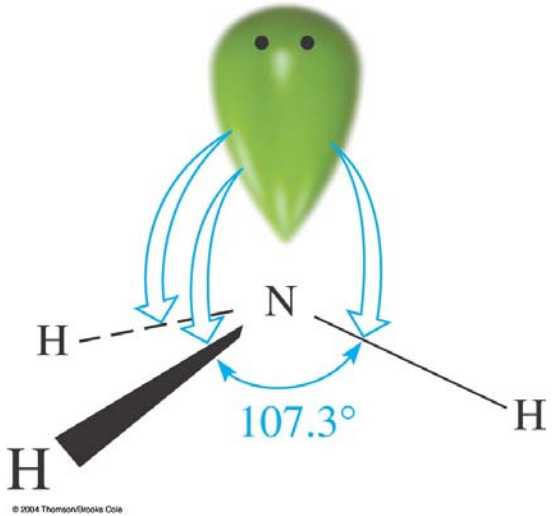
  All three substituents are the same but molecule is ***polar***.

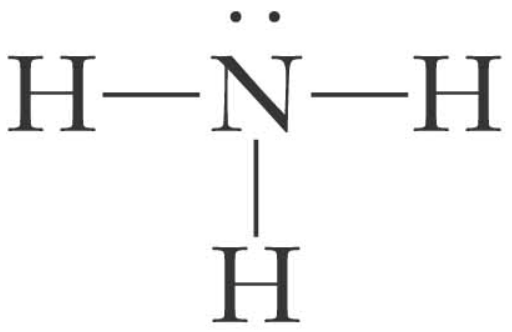
- NH_3 and NF_3 are trigonal pyramidal, polar molecules.

Tetrahedral Electronic Geometry: AB_3U Species (One Lone Pair of Electrons on A)

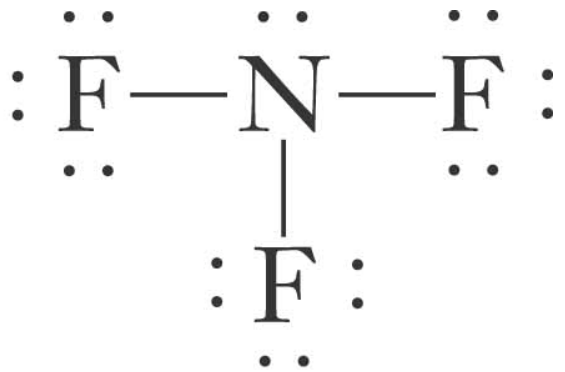
Valence Bond Theory



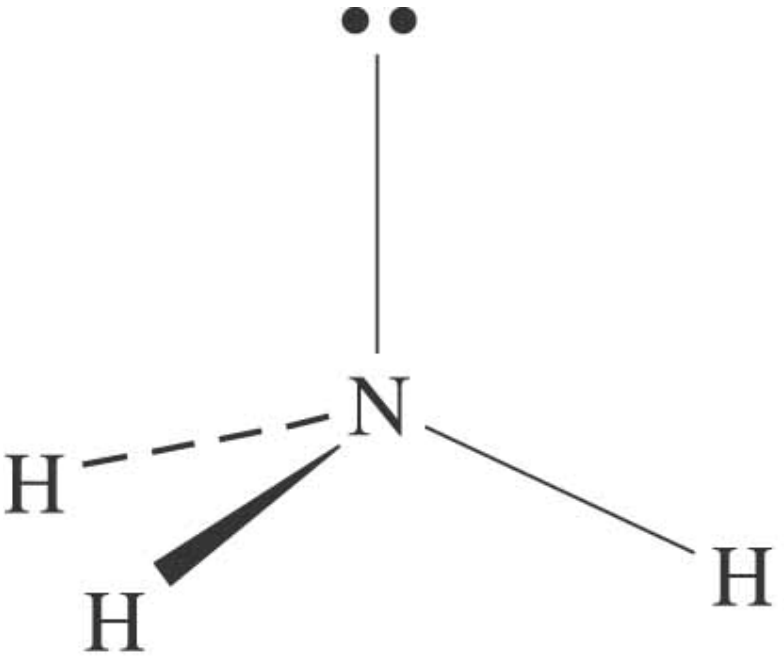


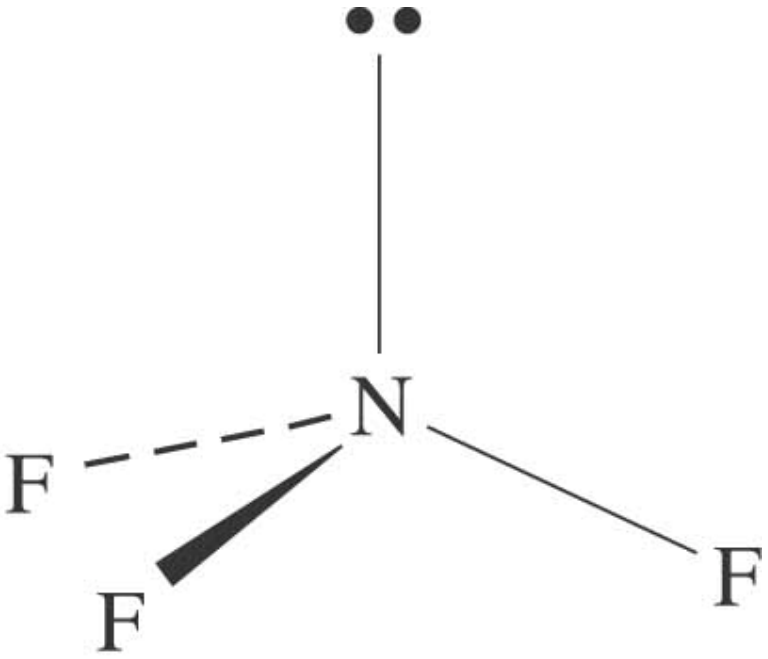


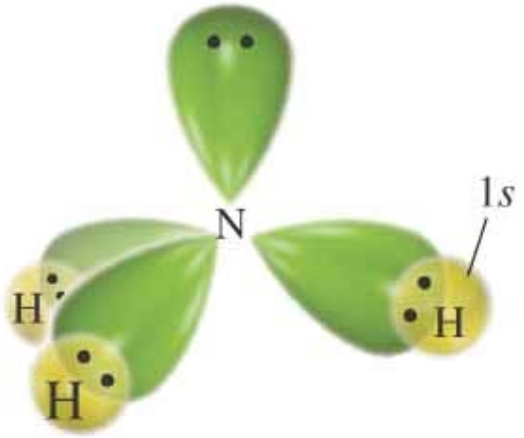
NH_3

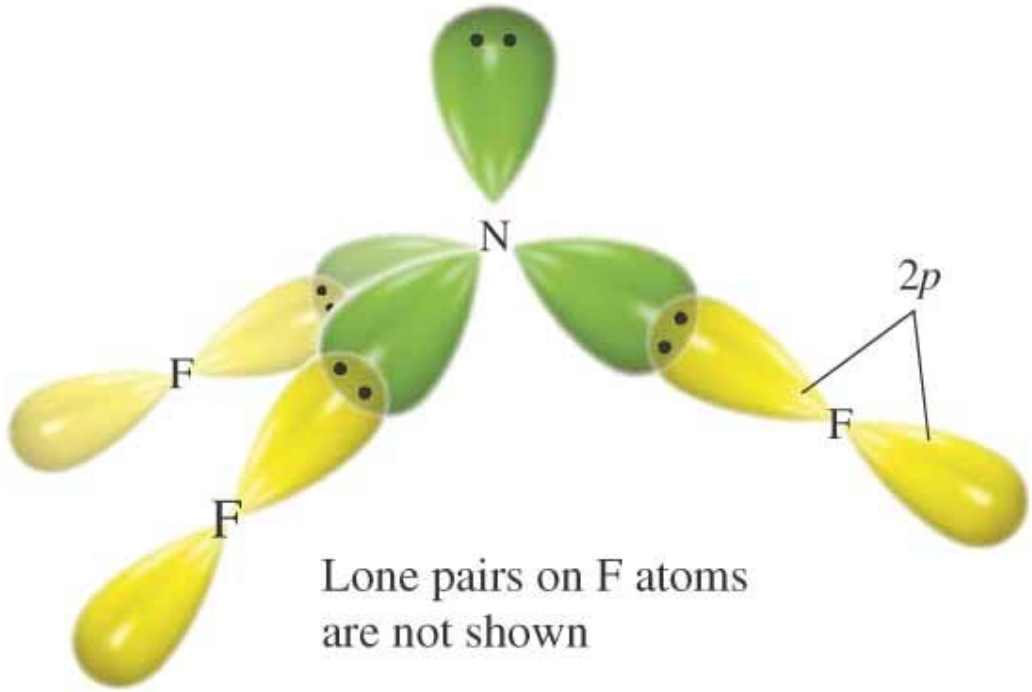


NF_3

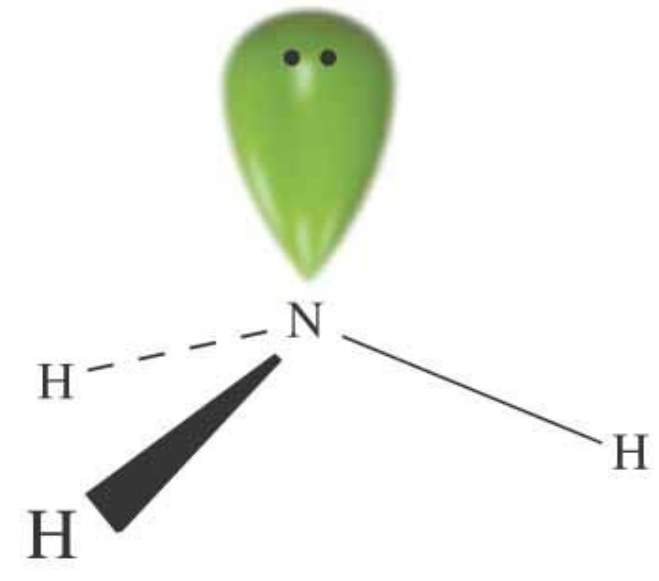








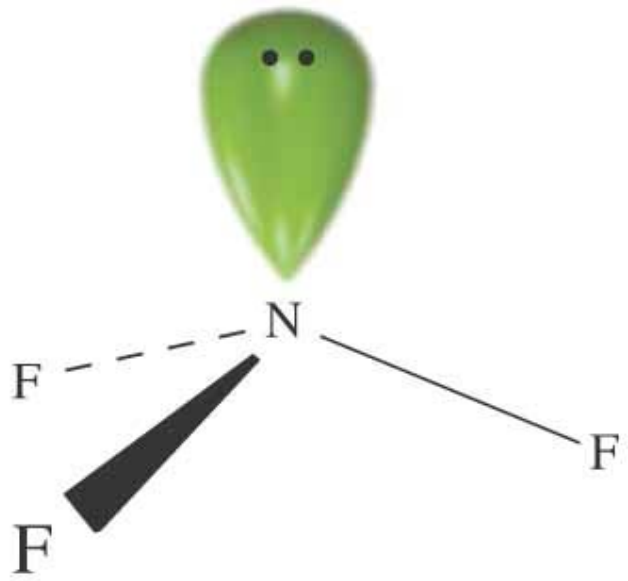
Molecular and Electronic Geometry



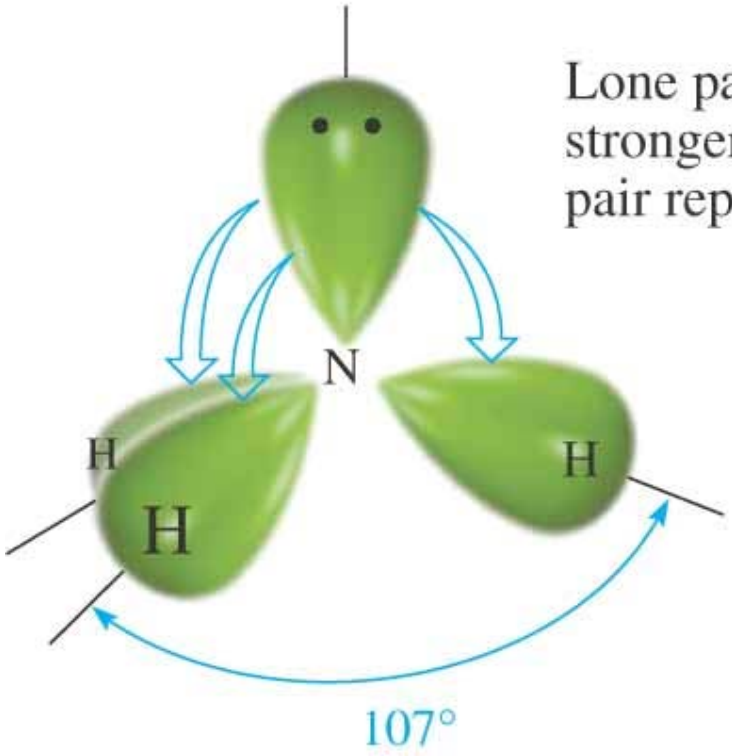
In NH_3, H–N–H angle = 107.3°

Tetrahedral
electronic geometry

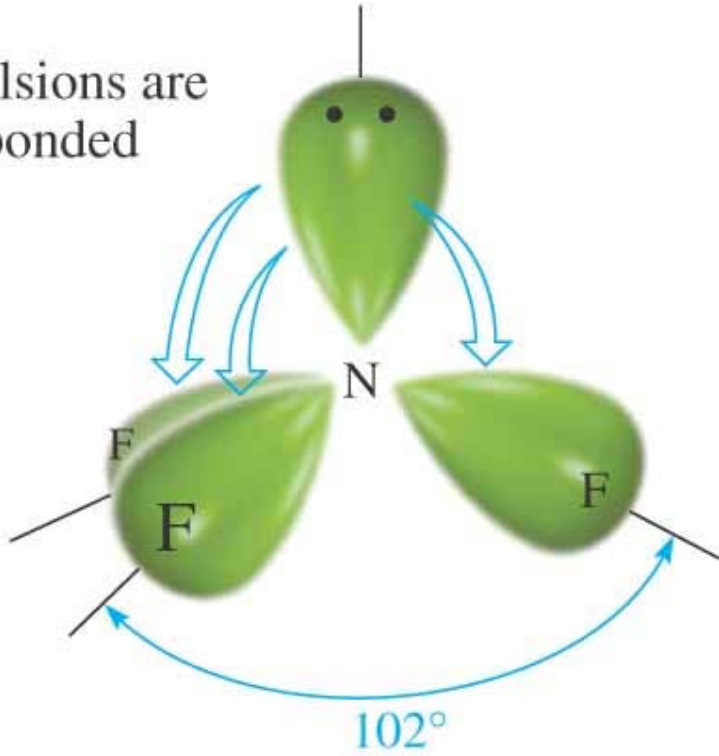
Trigonal pyramidal
molecular geometry



In NF_3, F–N–F angle = 102.1°

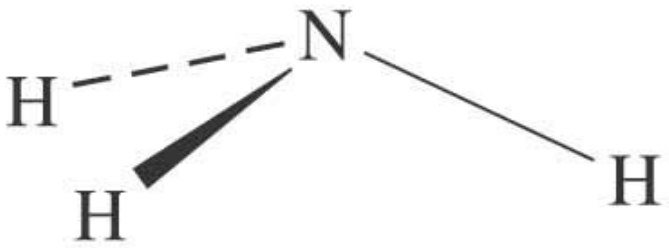


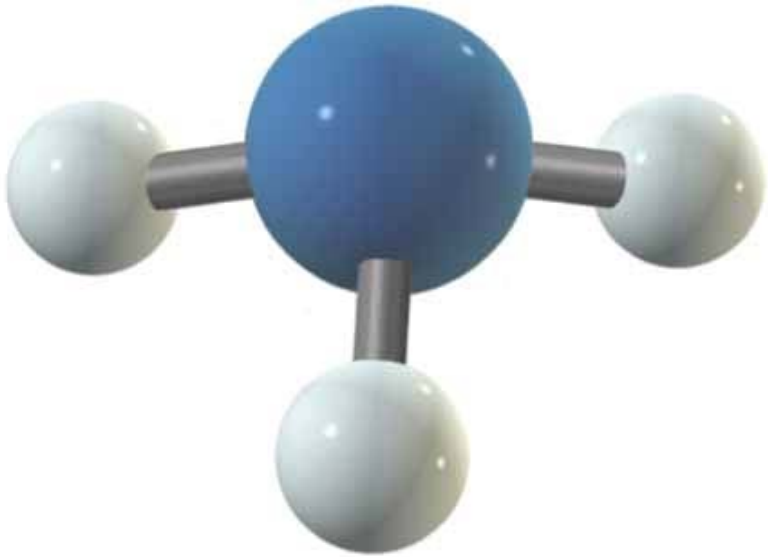
Lone pair/bonded pair repulsions are stronger than bonded pair/bonded pair repulsions

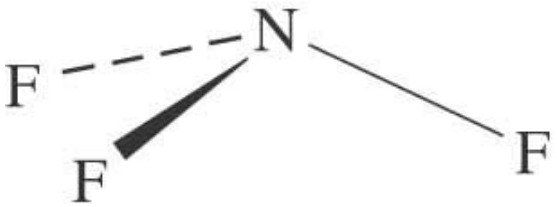


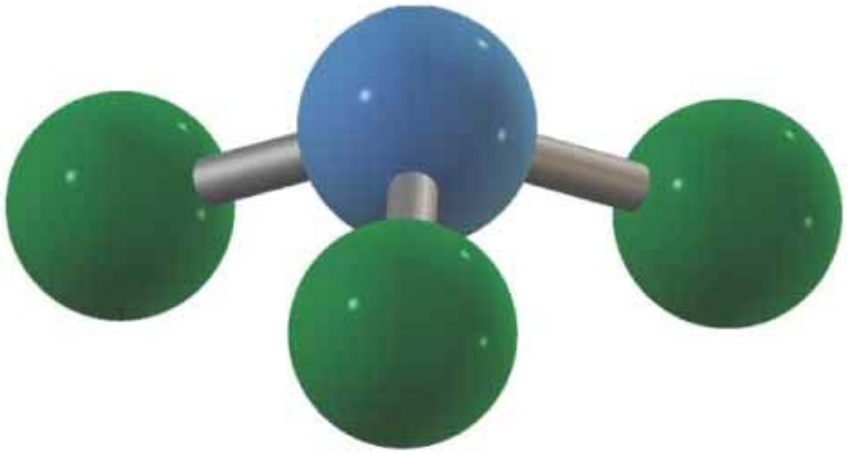
Bonded pair/bonded pair repulsions are weaker in NF_3 than in NH_3 due to the longer N—F bond

Molecular Geometry



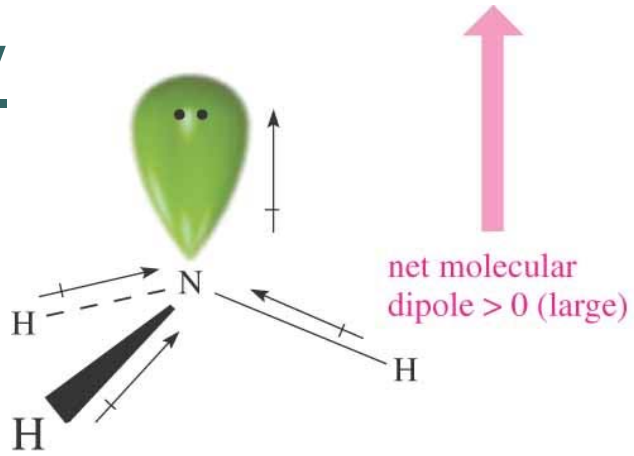


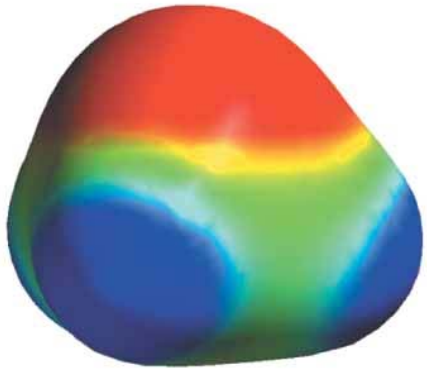


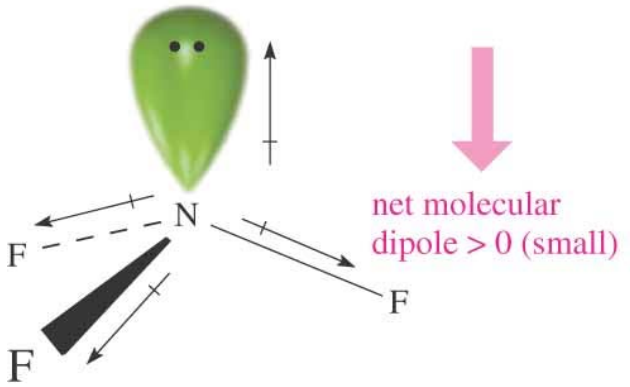


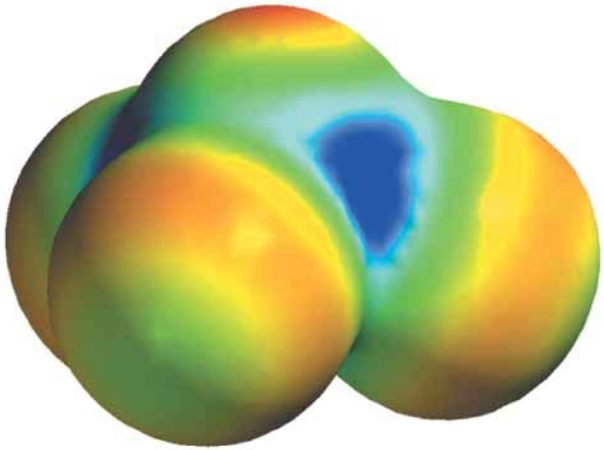
Tetrahedral Electronic Geometry: AB_3U Species (One Lone Pair of Electrons on A)

Polarity









Tetrahedral Electronic Geometry: AB_2U_2 Species (Two Lone Pairs of Electrons on A)

- Some examples of molecules with this geometry are:

  H_2O, OF_2, OCl_2, H_2S

- These molecules are our first examples of central atoms with two lone pairs of electrons.

  Thus, the electronic and molecular geometries are different.

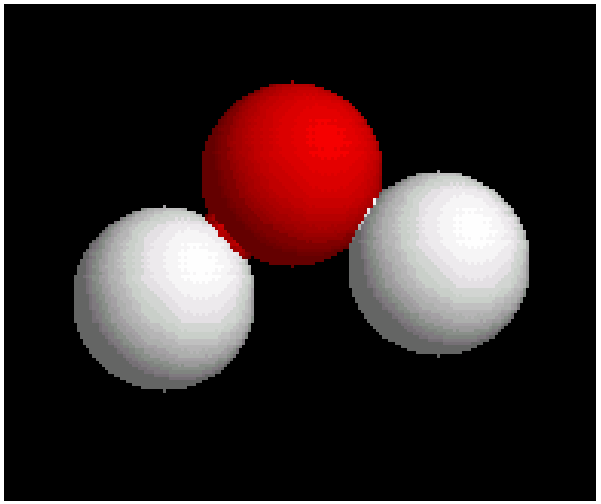
  Both substituents are the same but molecule is ***polar***.

- **Molecules are angular, bent, or V-shaped and polar.**

Tetrahedral Electronic Geometry: AB_2U_2 Species (Two Lone Pairs of Electrons on A)

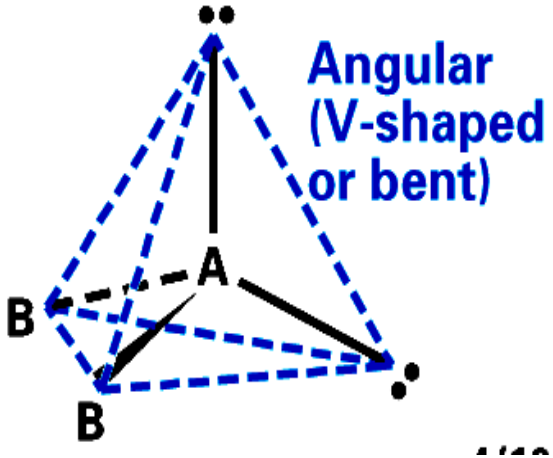
Valence Bond Theory (Hybridization)

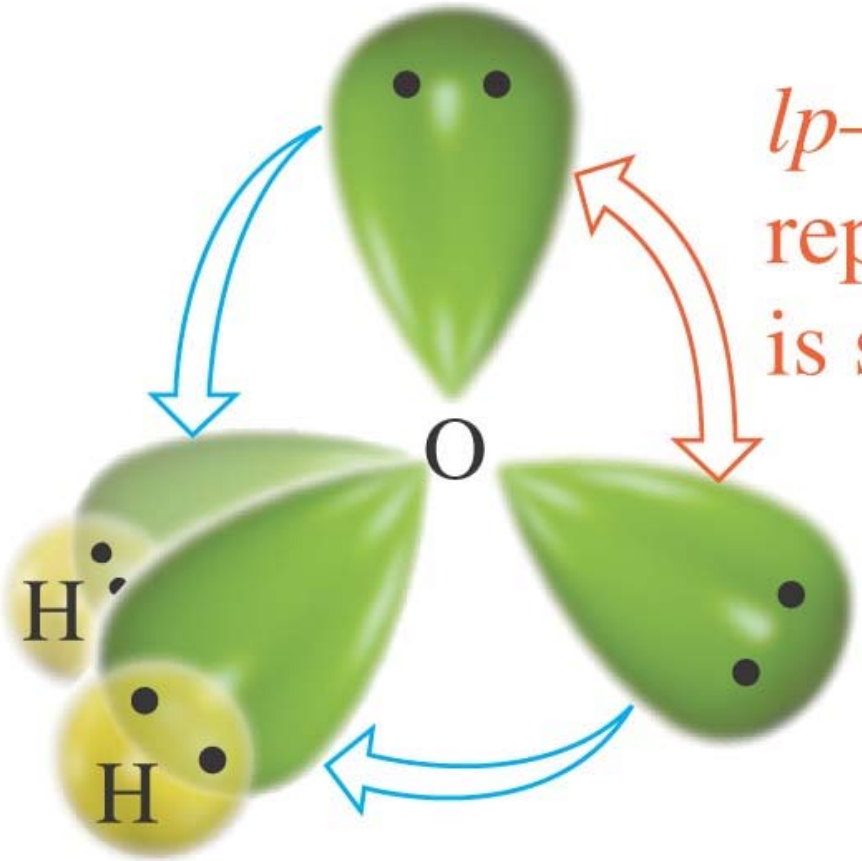
	2s	2p		four sp^3 hybrids
O [He]	↑↓	↑↓ ↑ ↑	⇒	↑↓ ↑↓ ↑ ↑



sp^3

2 unshared pairs





lp–lp repulsion is strongest

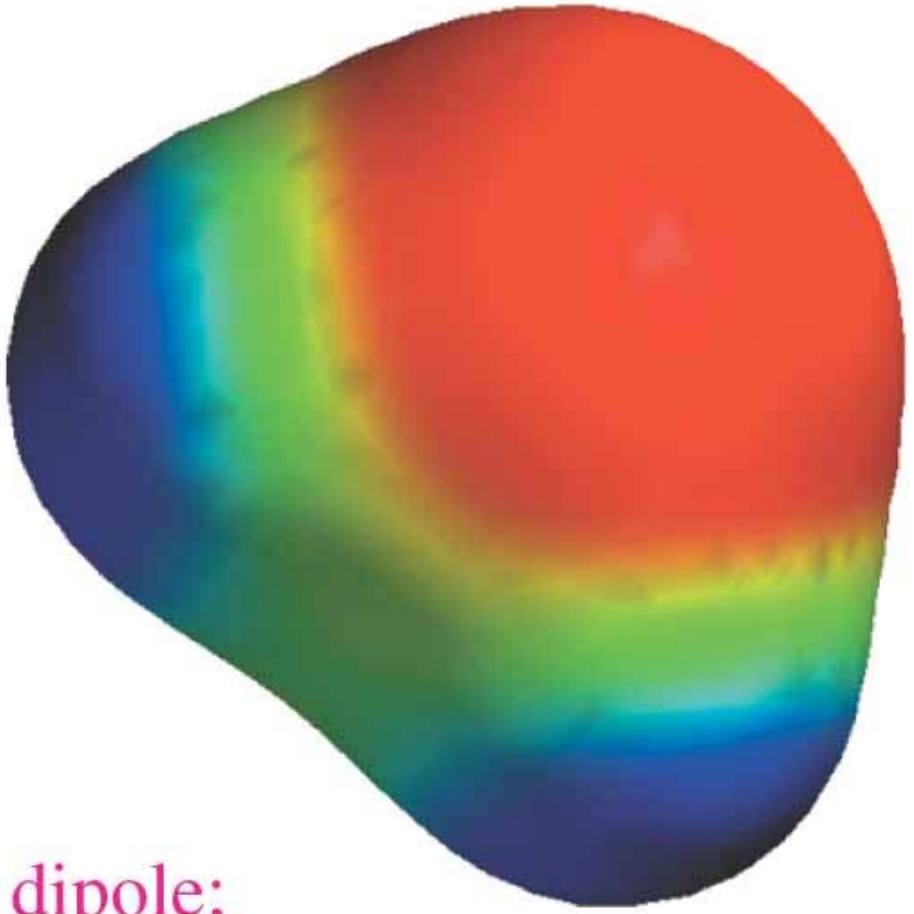
There are now *two* lone pairs that repel the bonded pairs

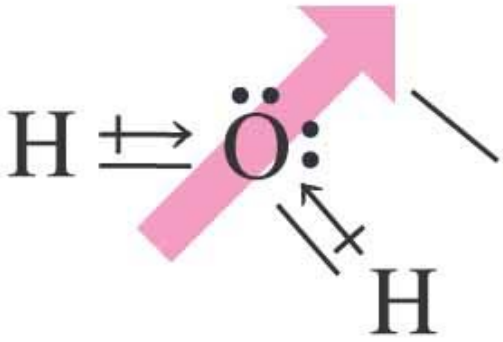
Polarity

O—H

EN = 3.5 2.1

$\Delta(EN) = 1.4$





Molecular dipole; includes effect of two unshared electron pairs

Tetrahedral Electronic Geometry: ABU_3 Species (Three Lone Pairs of Electrons on A)

- Some examples of molecules with this geometry are:

  HF, HCl, HBr, HI, FCl, IBr

- These molecules are examples of central atoms with three lone pairs of electrons.

  Again, the electronic and molecular geometries are different.

- Molecules are linear and polar when the two atoms are different.

  Cl_2, Br_2, I_2 are nonpolar.

Tetrahedral Electronic Geometry: ABU_3 Species (Three Lone Pairs of Electrons on A)

Dot Formula (HF)

Electronic Geometry (HF)

Tetrahedral Electronic Geometry: ABU_3 Species (Three Lone Pairs of Electrons on A)

Molecular Geometry (HF)

Polarity (HF)

Tetrahedral Electronic Geometry: ABU_3 Species (Three Lone Pairs of Electrons on A)

Valence Bond Theory (Hybridization)

Trigonal Bipyramidal Electronic Geometry: AB_5, AB_4U, AB_3U2, and AB_2U_3

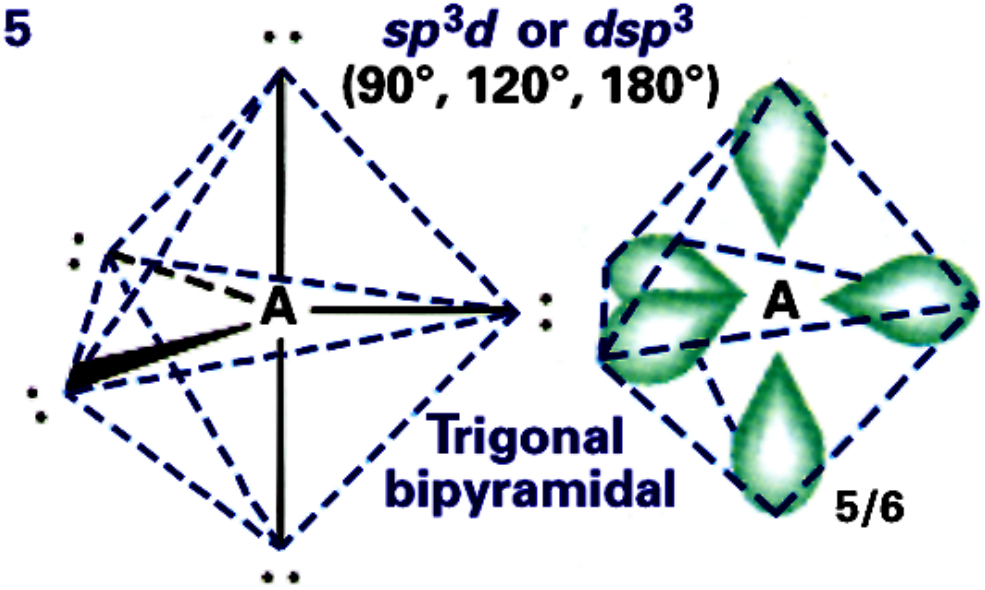
- Some examples of molecules with this geometry are:
  PF_5, AsF_5, PCl_5, etc.
- These molecules are examples of central atoms with five bonding pairs of electrons.
  The electronic and molecular geometries are the same.
- Molecules are trigonal bipyramidal and nonpolar when all five substituents are the same.
  If the five substituents are not the same, **polar** molecules can result, AsF_4Cl is an example.

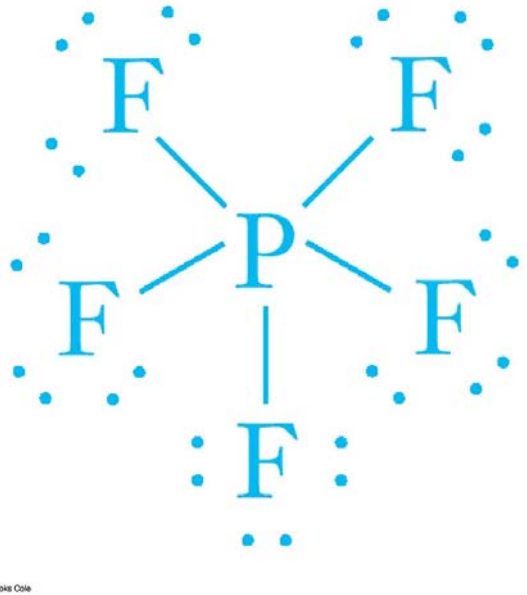
Trigonal Bipyramidal Electronic Geometry: AB_5, AB_4U, AB_3U2, and AB_2U_3

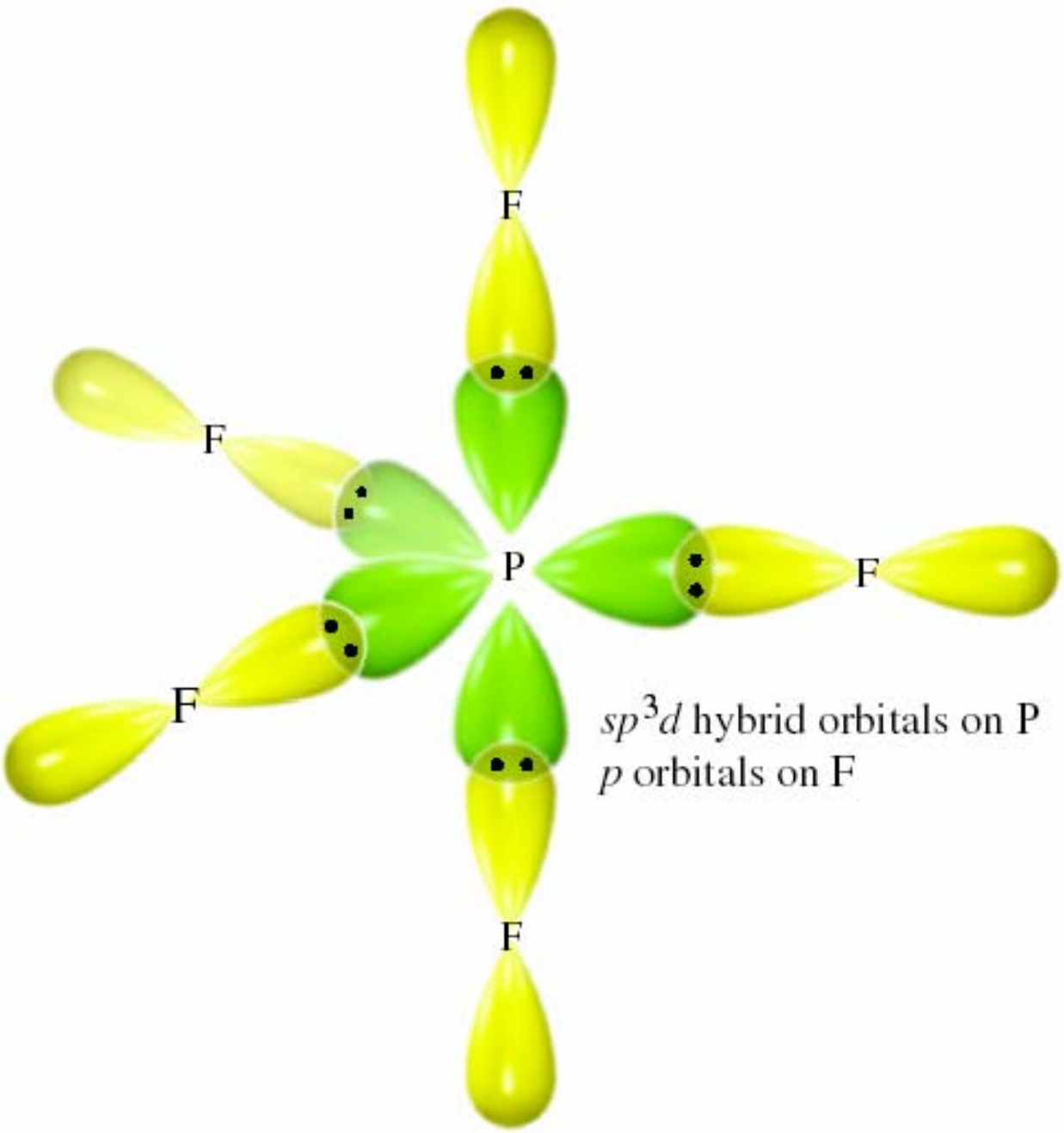
Valence Bond Theory

Trigonal Bipyramidal Electronic Geometry: AB_5, AB_4U, AB_3U2, and AB_2U_3

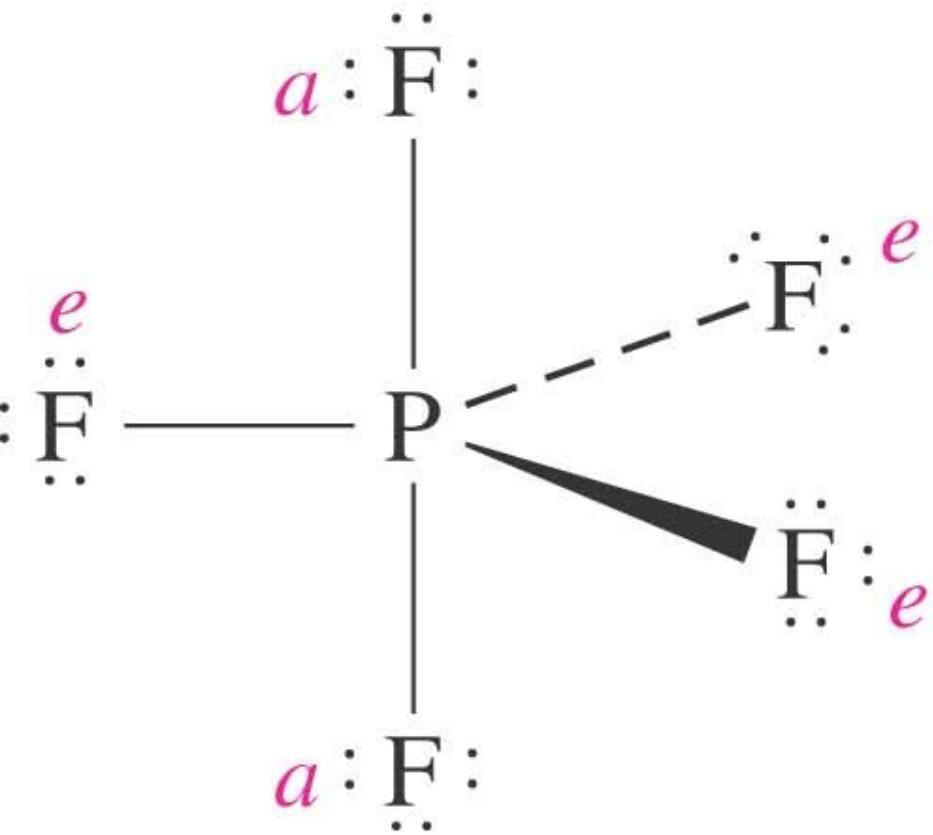
Regions of high electron density	Electronic geometry	Hybridization at central atom (angle)	Hybridized orbital orientation
5	Trigonal bipyramidal	sp^3d or dsp^3 (90°, 120°, 180°)	5/6

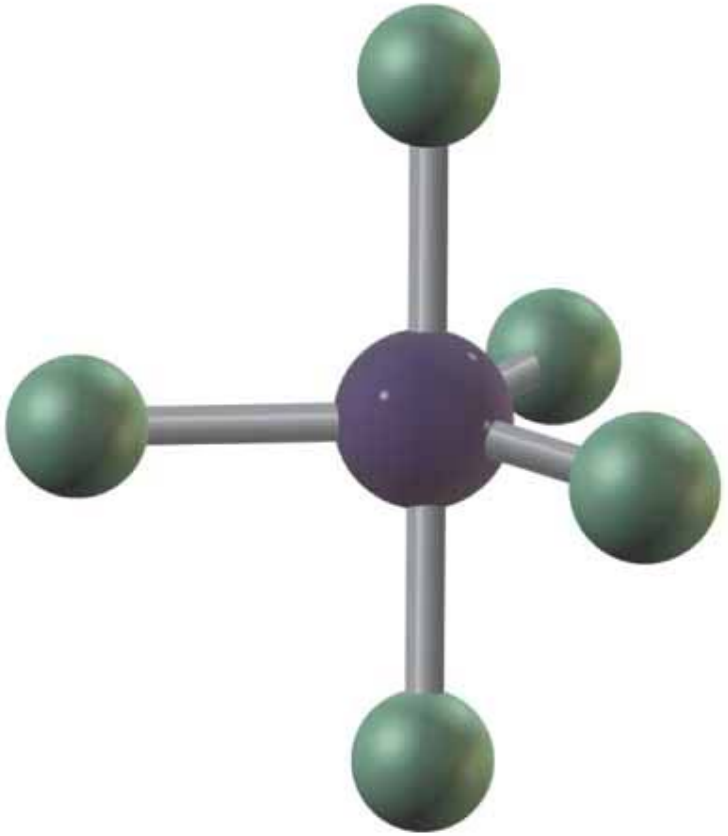





F
F
P
F
F
F
sp^3d hybrid orbitals on P
p orbitals on F

Molecular Geometry





Trigonal Bipyramidal

Polarity

	P—F
EN =	2.1 4.0
Δ(EN) =	1.9