VSEPR

Valence Shell Electron Pair Repulsion Theory

Vocabulary:

“domain”

= any electron pair **or** bond (single, double or triple) is considered one domain.

“lone pair” = “non-bonding pair” = “unshared pair”
= any electron pair that is not involved in bonding

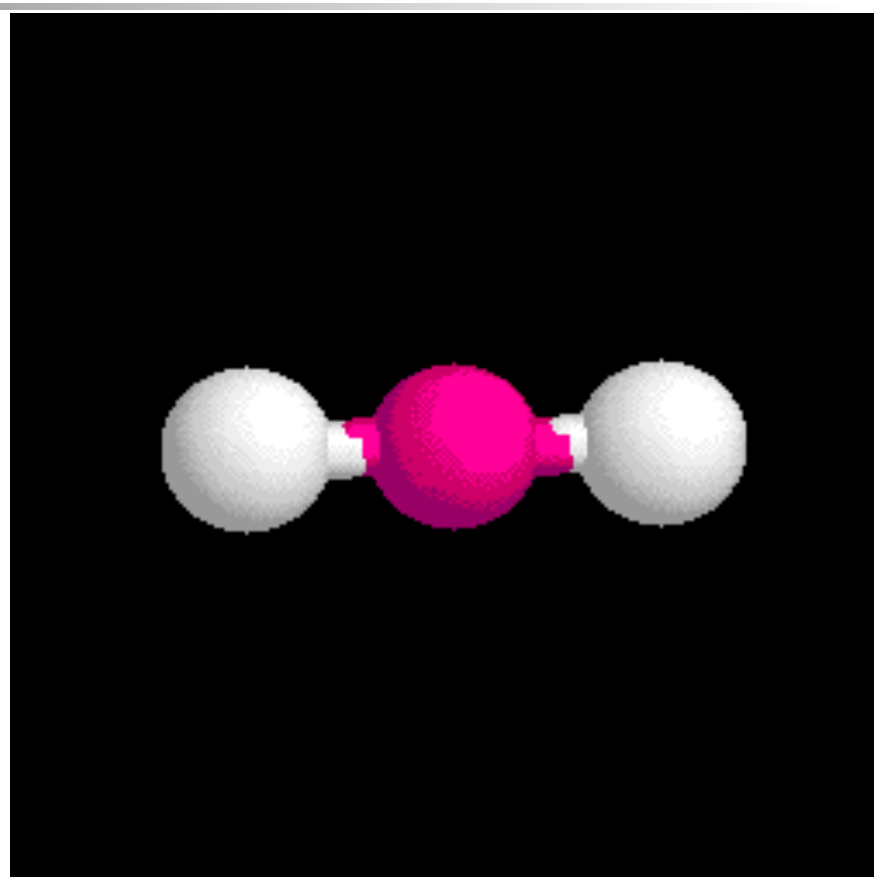
“bonding pair” = “shared pair”
= any electron *pair* that is involved in bonding

2 domains on central atom

LINEAR

- 2 domains
- both are bonding pairs

- They push each other to opposite sides of center (180° apart).

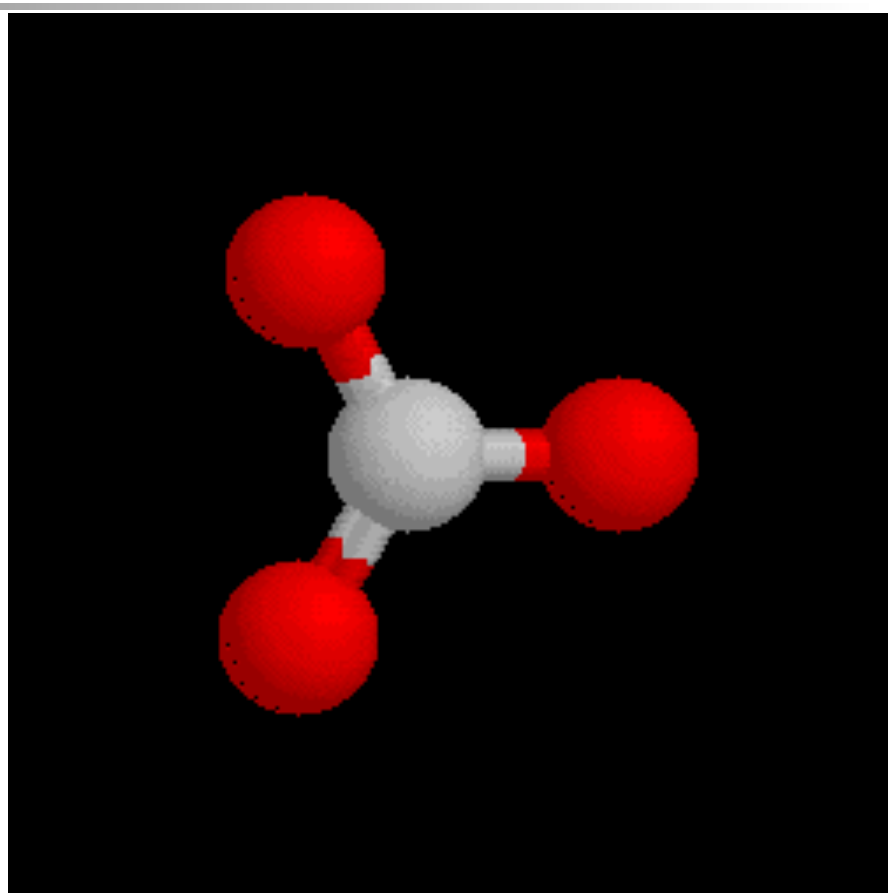


$BeCl_2$

3 domains on central atom

TRIGONAL PLANAR

- 3 domains
- all are bonding pairs
- They push each other apart equally at 120° degrees.

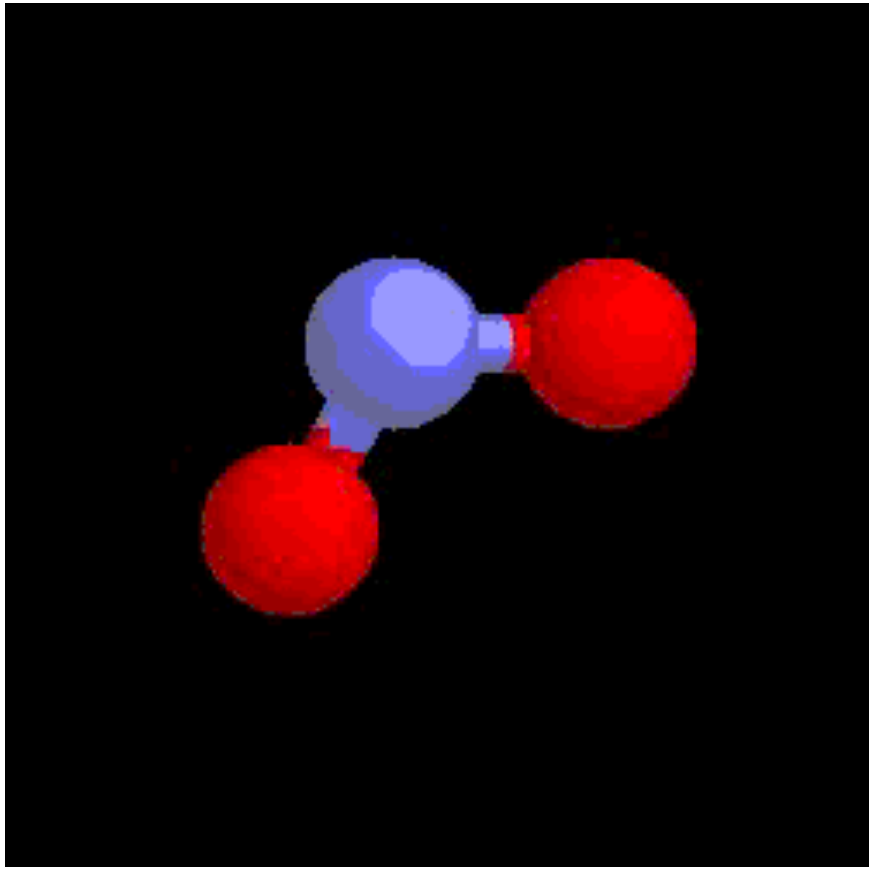


GaF_3

3 domains on central atom

BENT

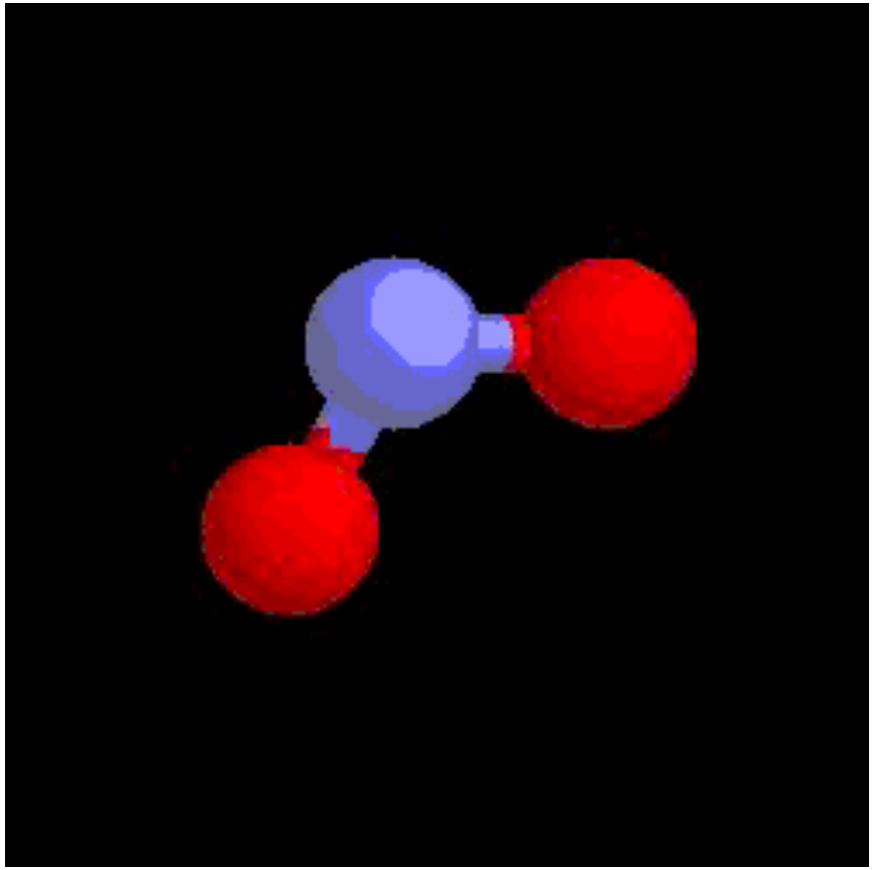
- 3 domains:
  - 2 are bonding pairs
  - 1 is a lone pair
- The 2 bonding pairs are pushed apart by 3rd pair (not seen)



SnF_2

NOTE:

- The *geometry around the central atom* is **trigonal planar.**
- The *molecular shape* is **bent**.

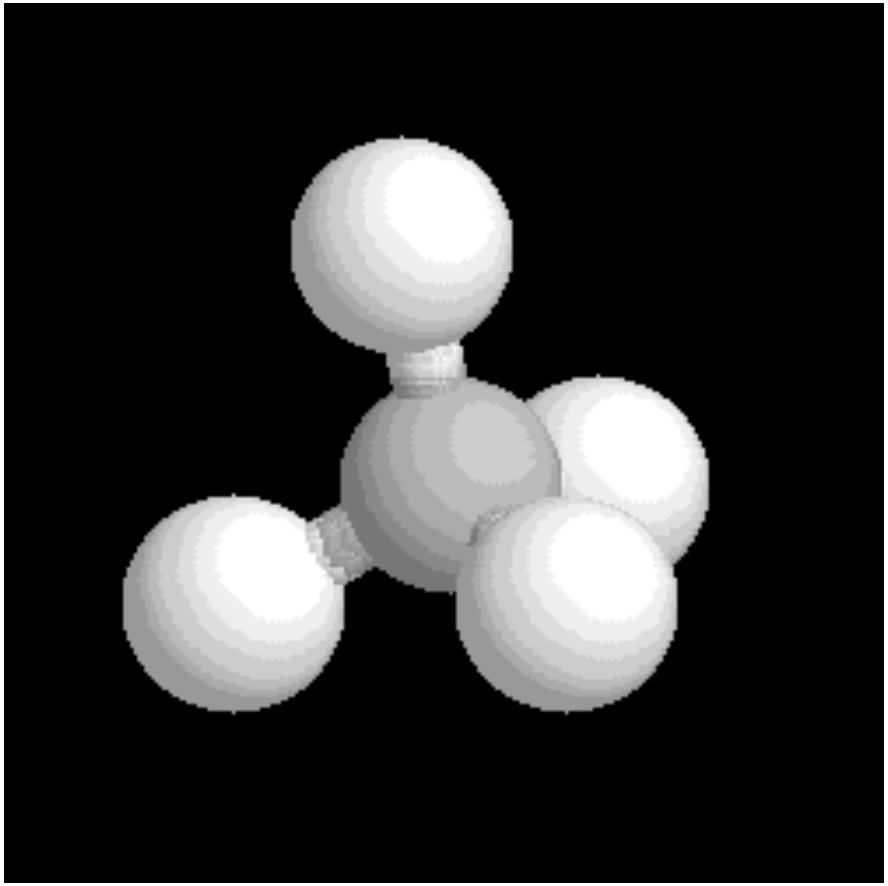


SnF_2

4 domains on central atom

TETRAHEDRAL

- 4 domains
- Each repels the other equally - 109.5° - **not** the expected 90°.
- *Think in 3D.*

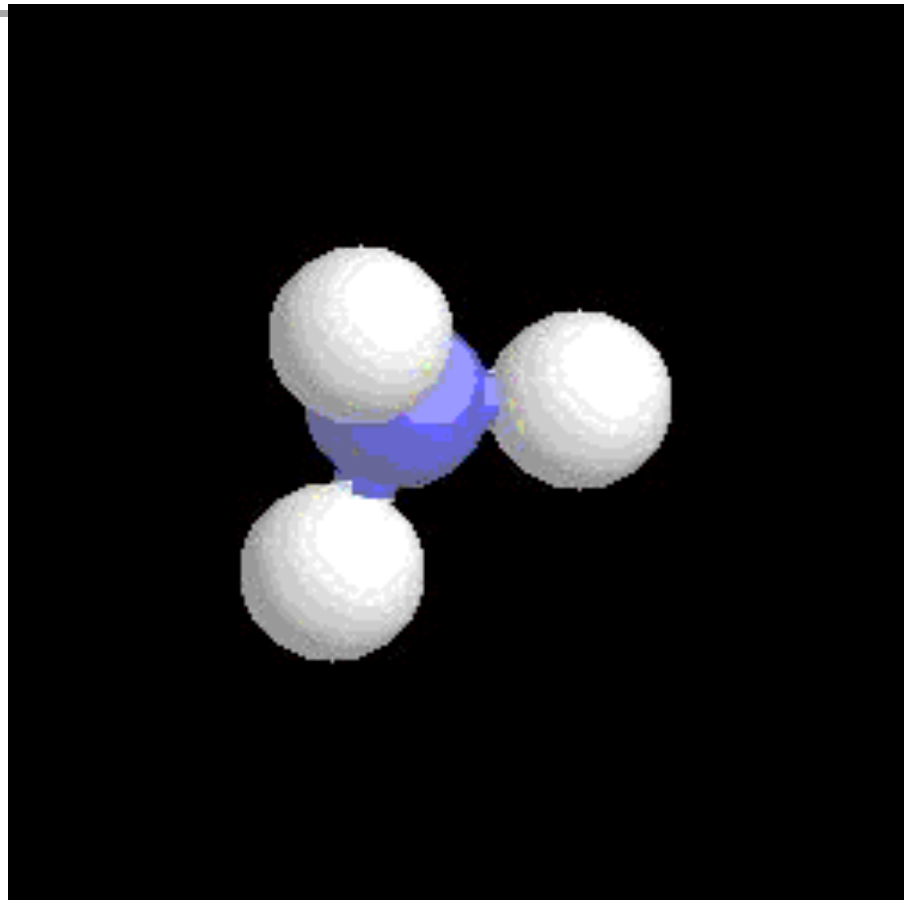


CH_4

4 e^- pairs on central atom

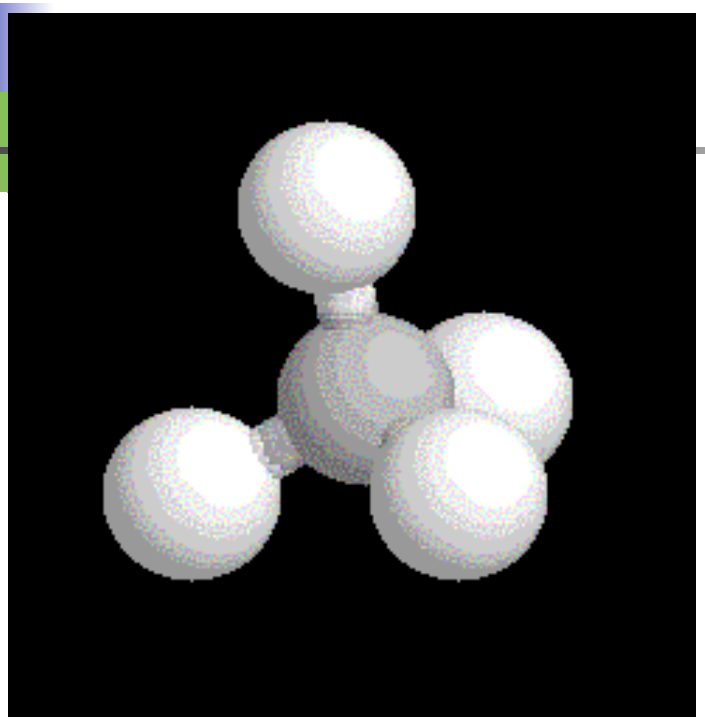
TRIGONAL PYRAMIDAL

- 4 domains
  - 3 bonding pairs
  - 1 lone pair
- The thicker, lone pair forces the others a little bit closer together (~107.3°)



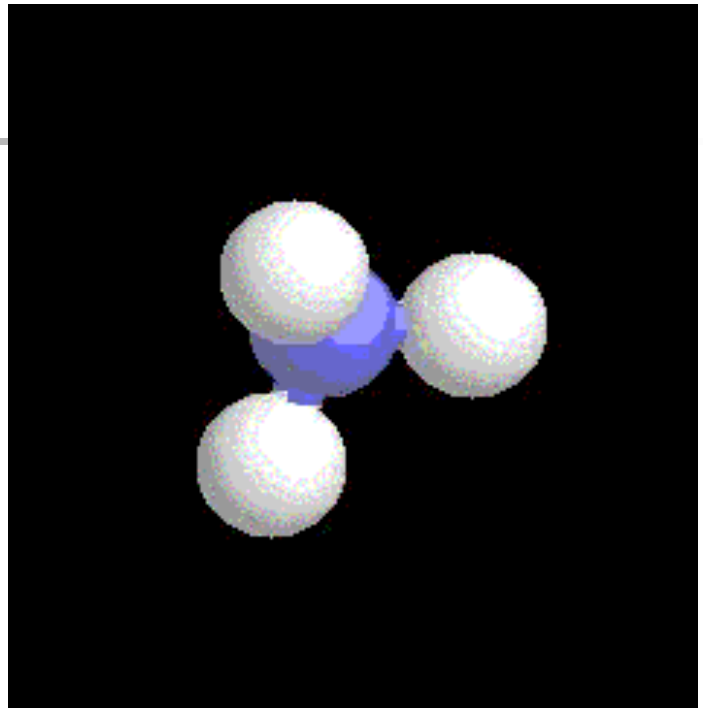
NH_3

Tetrahedral *vs.* Trigonal pyramidal



Tetrahedral *geometry around the central atom*

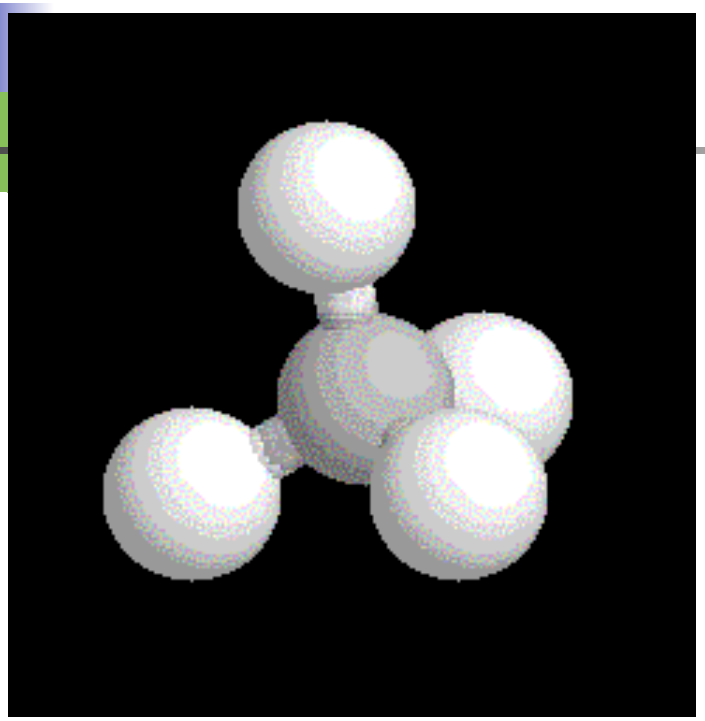
Tetrahedral
Molecular Shape

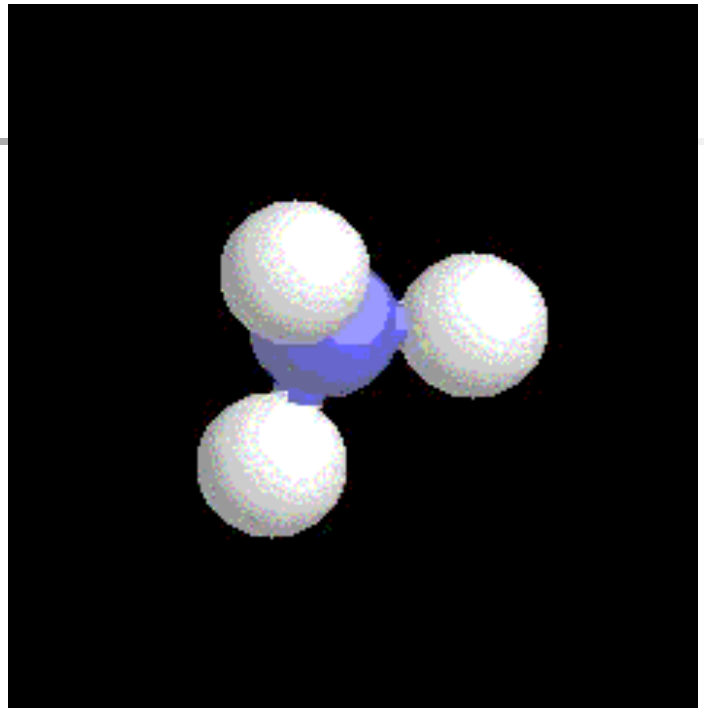


Tetrahedral *geometry around the central atom*

Trigonal Pyramidal
Molecular Shape

Tetrahedral *vs.* Trigonal pyramidal





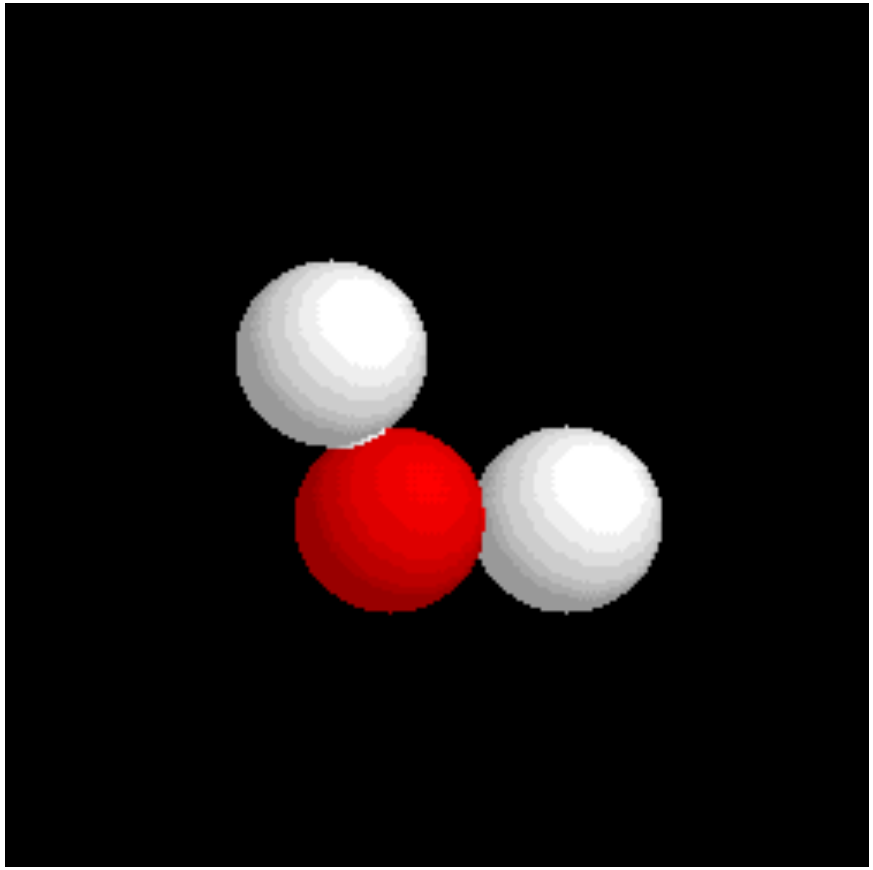
On the right, the 4th lone pair, is not seen as part of the actual molecule, yet affects shape.

If another one of the bonding pairs on “trigonal pyramidal” were a lone pair, what is the result?

4 domains on central atom, con't

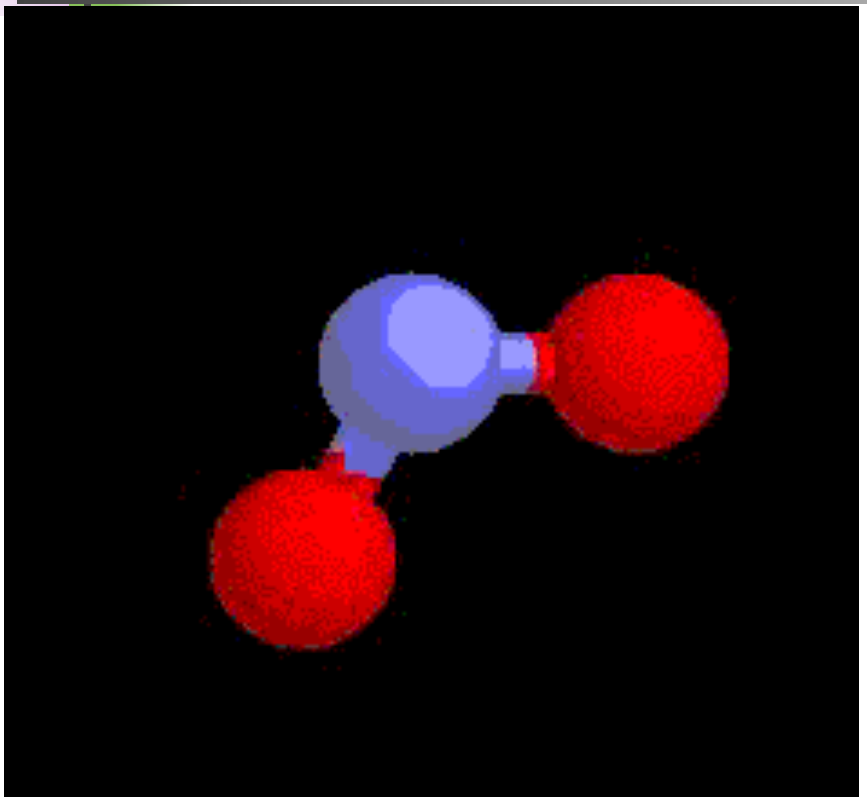
BENT

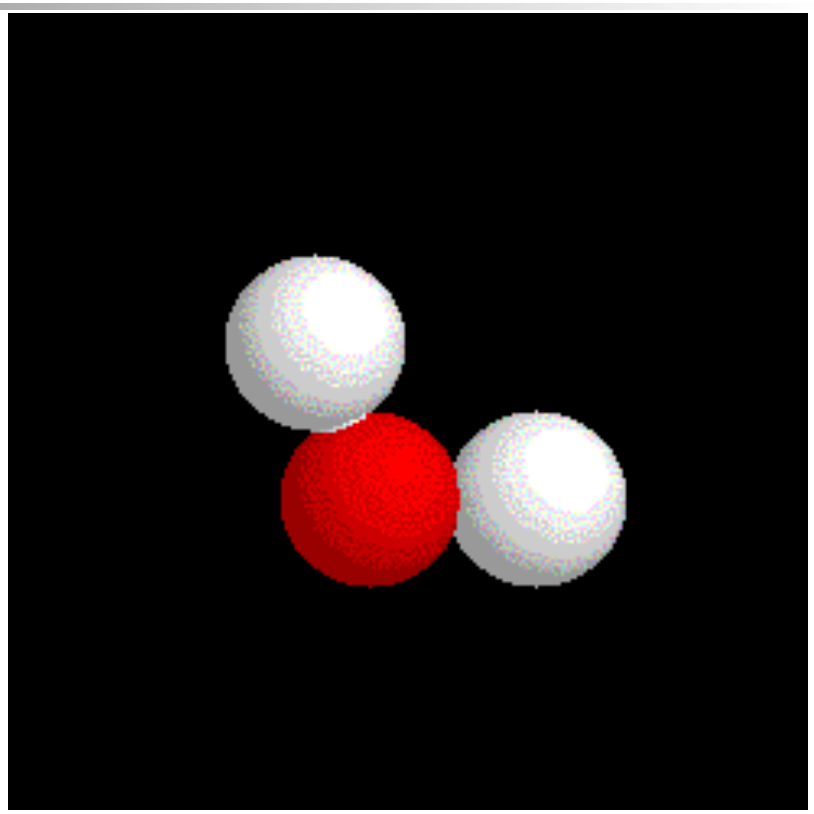
- 4 domains
  - 2 bonding pairs
  - 2 lone pairs
- The bonds are forced together still closer (104.5°) by the 2 thick unshared pairs.



H_2O

Comparing the 2 “bents”…





Both bent molecules are affected by unshared pairs – 1 pair on the left, 2 on the right.

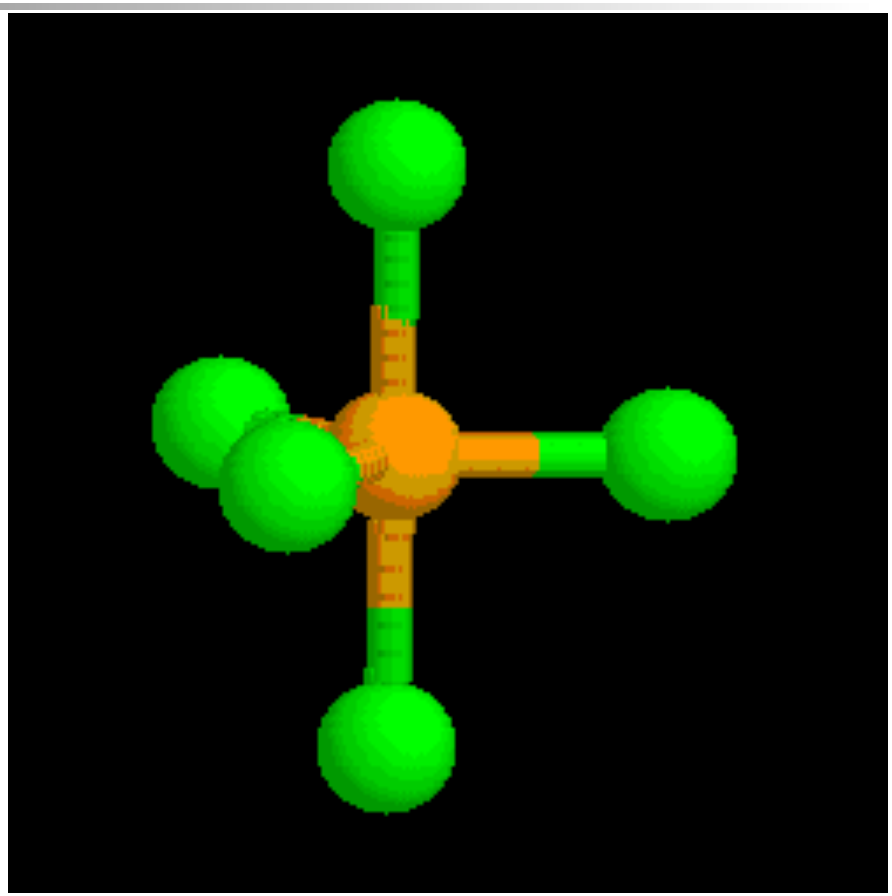
Other Molecular Geometry

Note that if there are more than five domains around the central atom, it must be an exception to the octet rule!

5 e^- pairs on central atom

TRIGONAL BIPYRAMIDAL

- 5 shared pairs
- Three pairs are found in one plane ("equator") 120° apart; the other two pairs are at the "poles," 180° apart, 90° from the "equator."

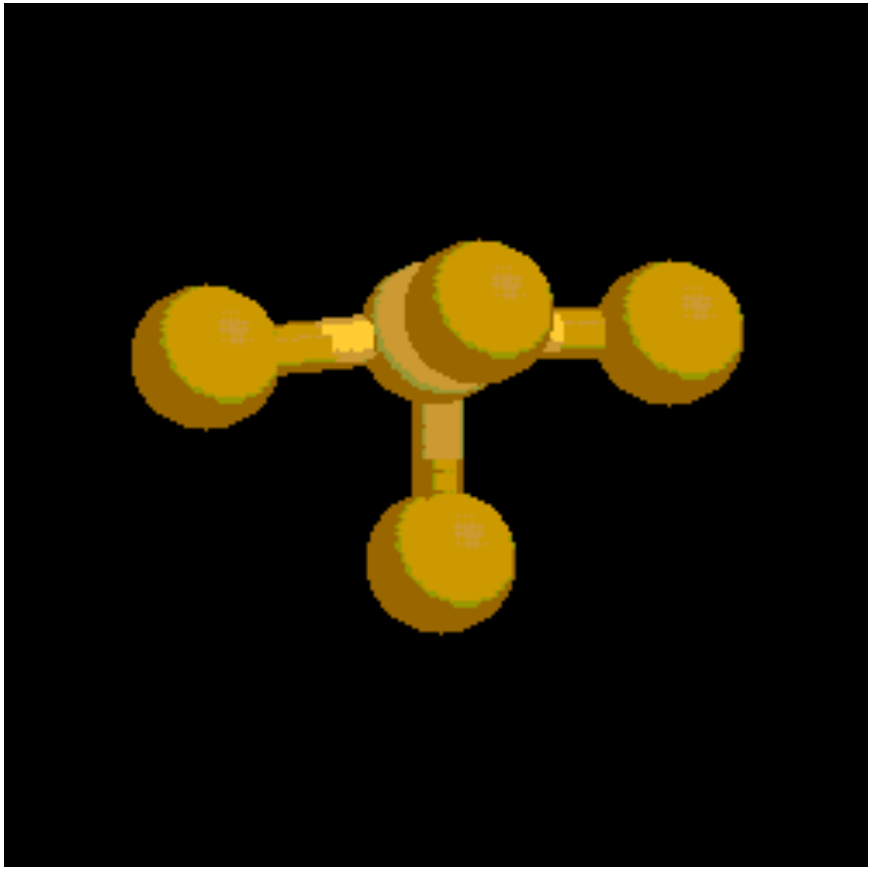


PCl_5

5 e^- pairs on central atom

SEE-SAW

- 4 shared pairs &
  1 unshared pair
- One of the equator pairs is unshared & pushes the other 2 together.
- The 2 poles are pushed slightly together.

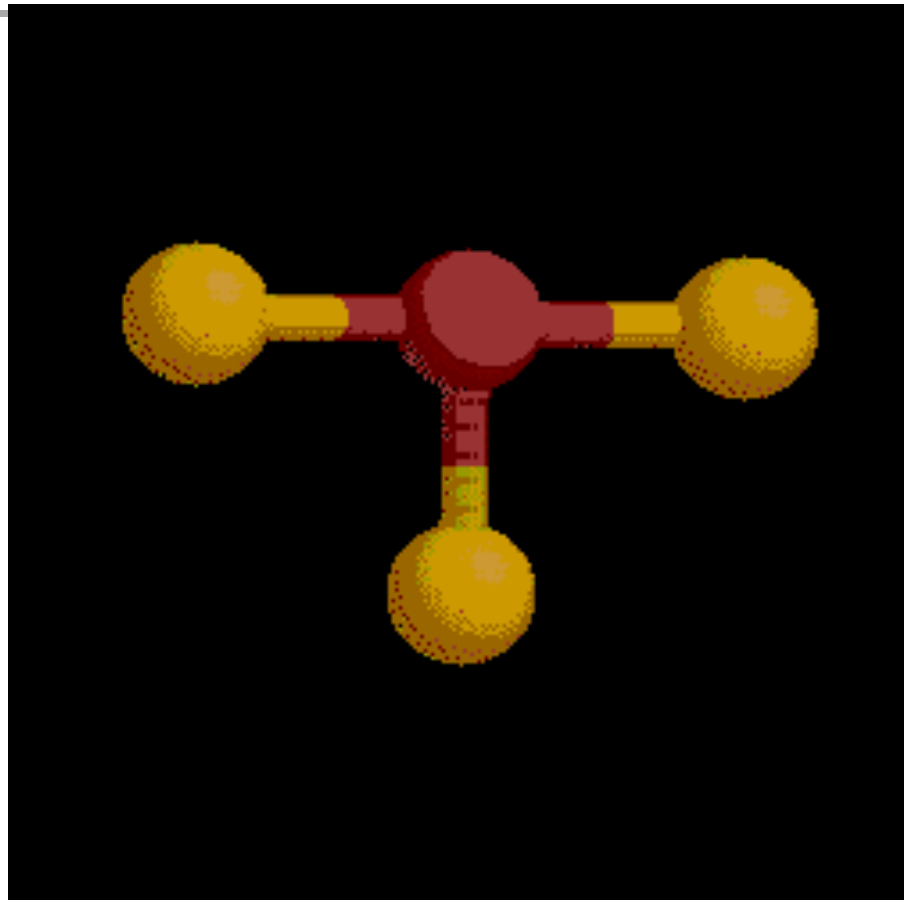


SF_4

5 e^- pairs on central atom

T-SHAPED

- 3 shared & 2 unshared pairs
- 2 of the 3 equator pairs are unshared.
- All 3 remaining pairs are pushed together.

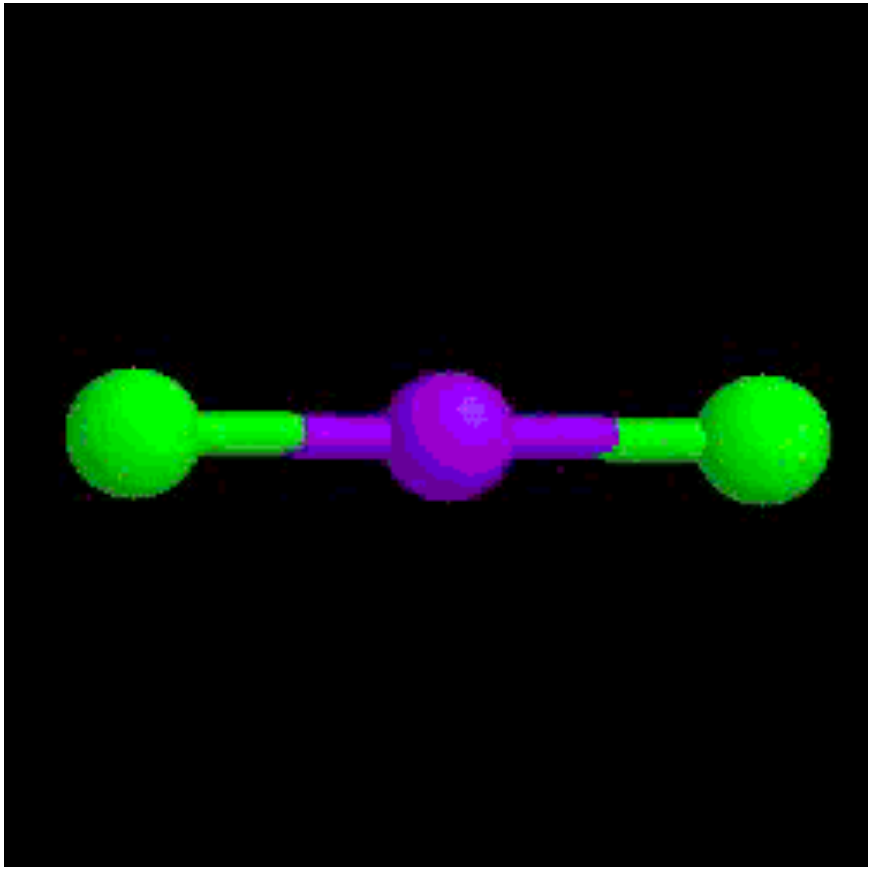


ClF_3

5 e^- pairs on central atom

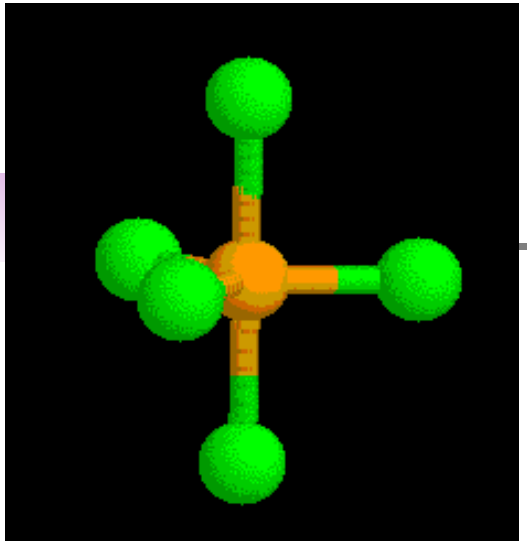
LINEAR

- 2 shared & 3 unshared pairs
- All 3 equator pairs are unshared. The 2 remaining pairs are forced to the poles.

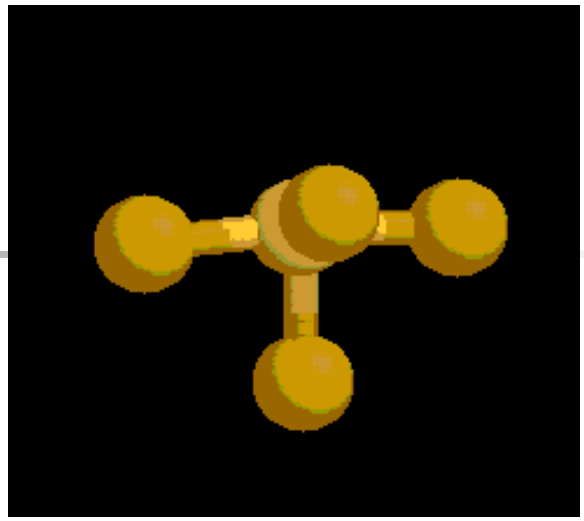


XeF_2

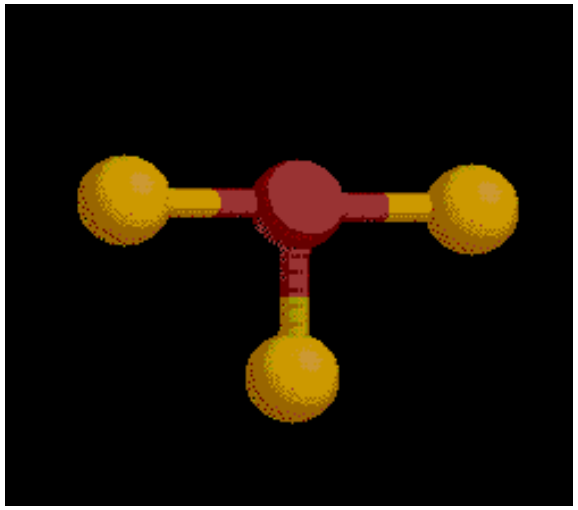
5 e^- pairs on central atom



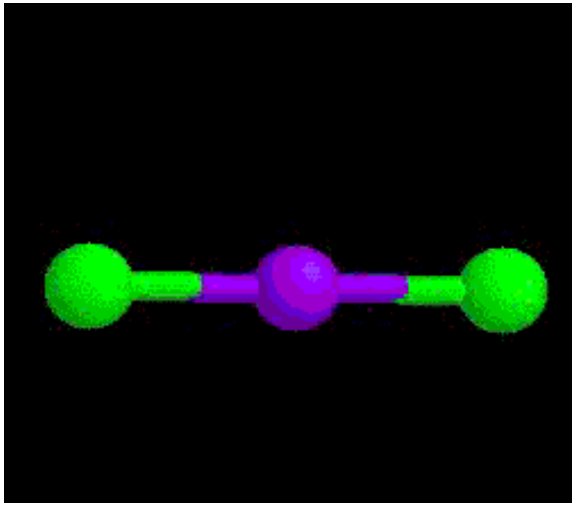
5 shared, 0 unshared



4 shared, 1 unshared



3 shared, 2 unshared



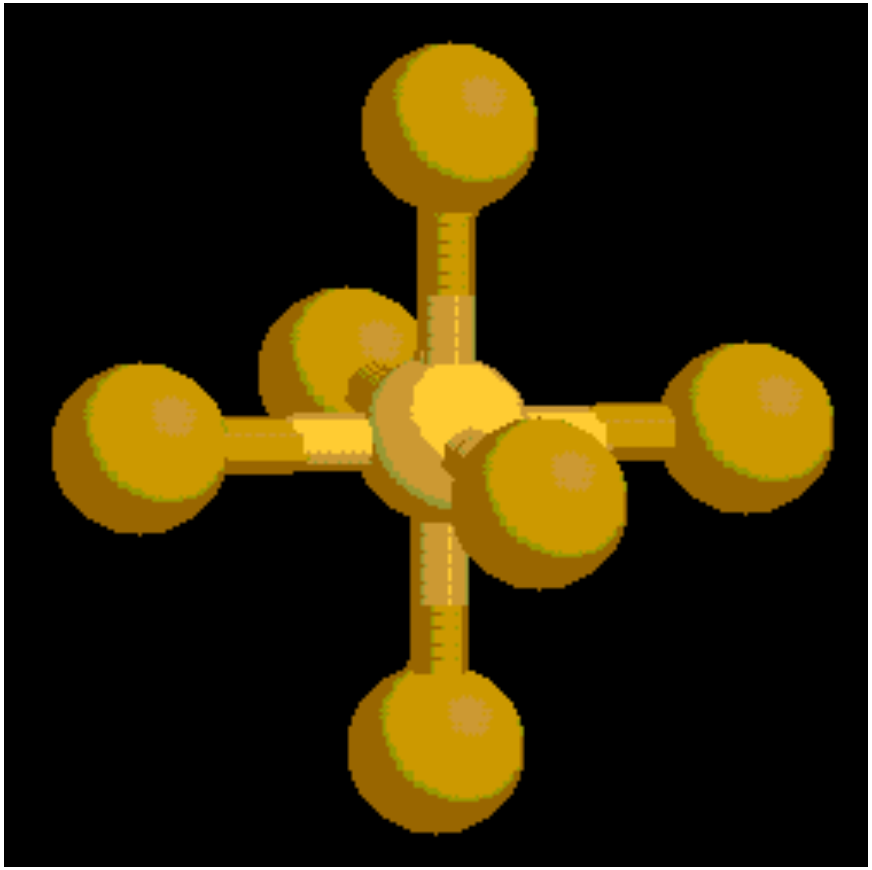
2 shared, 3 unshared

6 e^- pairs on central atom

OCTAHEDRAL

- 6 shared pairs
- Each pair repels the others equally.
- All angles = 90°

Now, if one of these pairs was unshared …



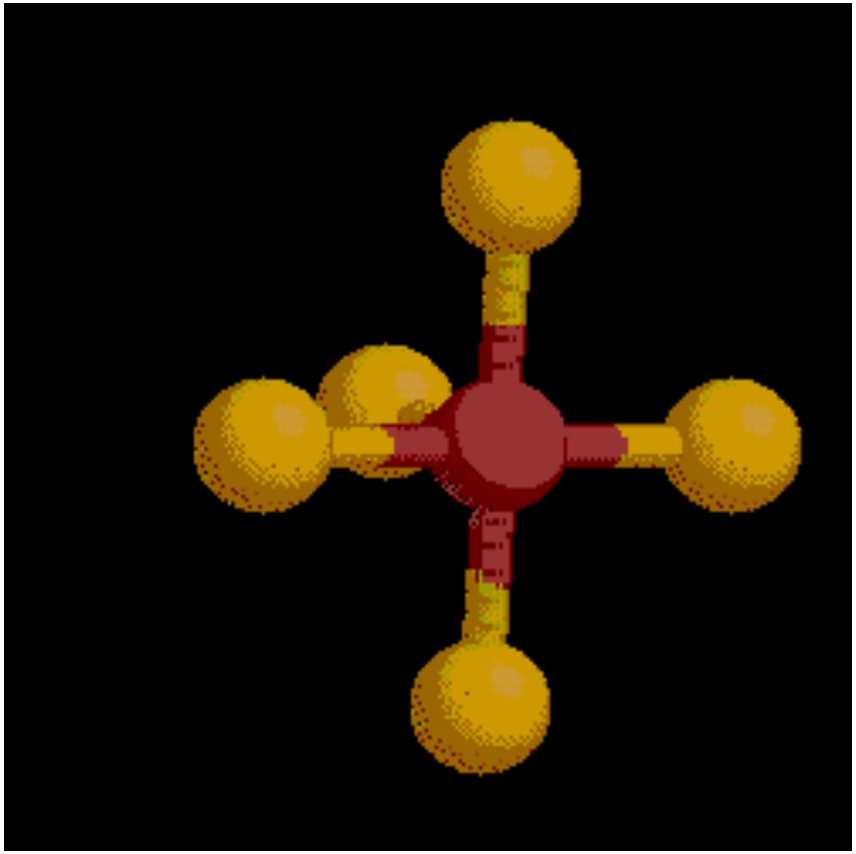
SF_6

6 e^- pairs on central atom

SQUARE PYRAMIDAL

- 5 shared pairs &
  1 unshared pair
- 4 shared pairs in one plane; the 5th pair at the pyramid's top.

If the pair at the top was unshared …

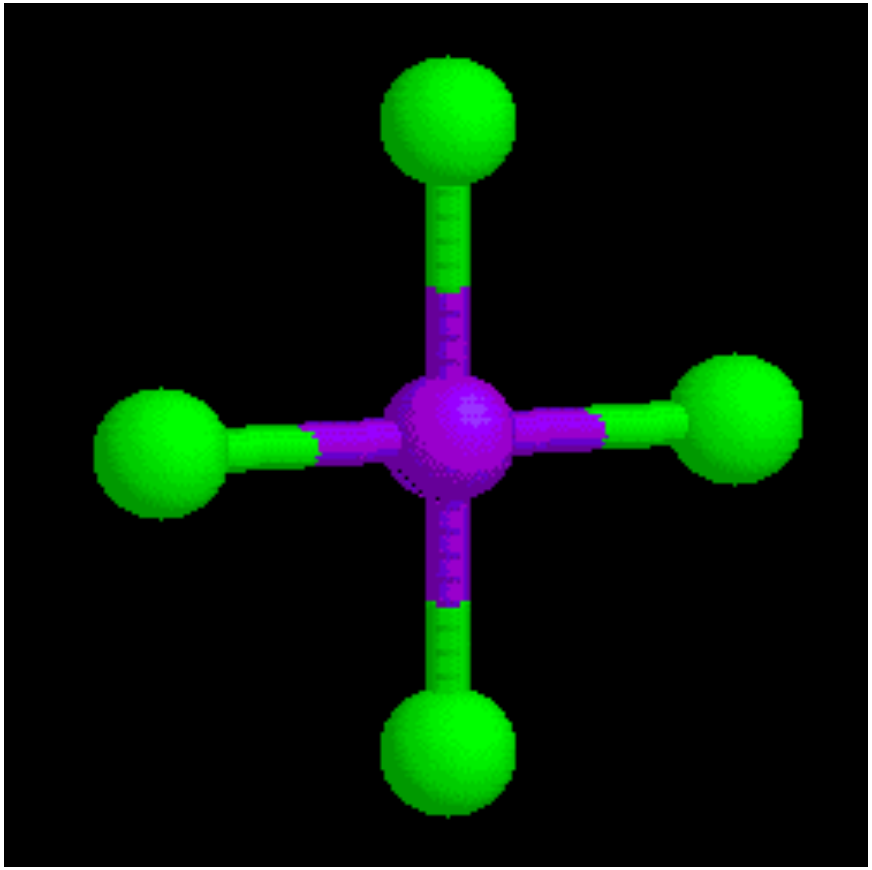


IF_5

6 e^- pairs on central atom

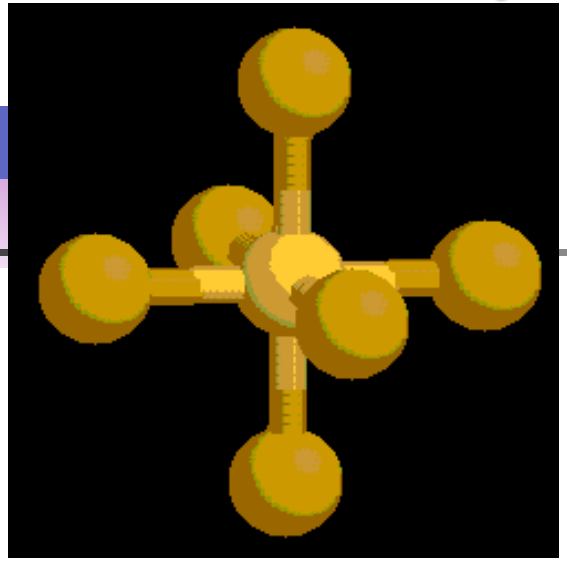
SQUARE PLANAR

- 4 shared & 2 unshared pairs
- The 4 shared pairs are in the same plane; the 2 unshared pairs are 90° from them.

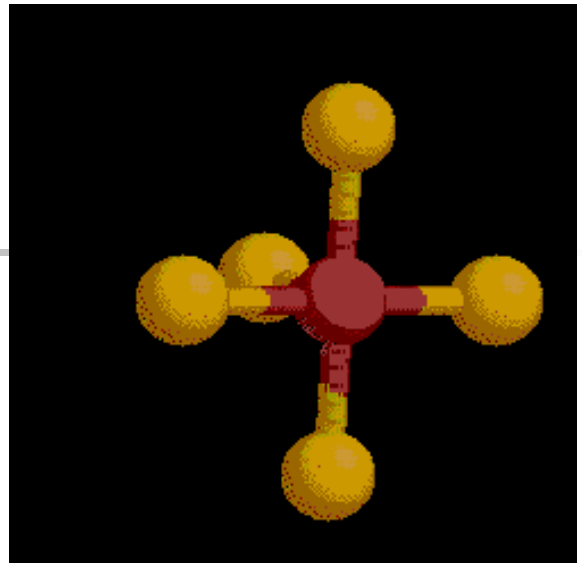


XeF_4

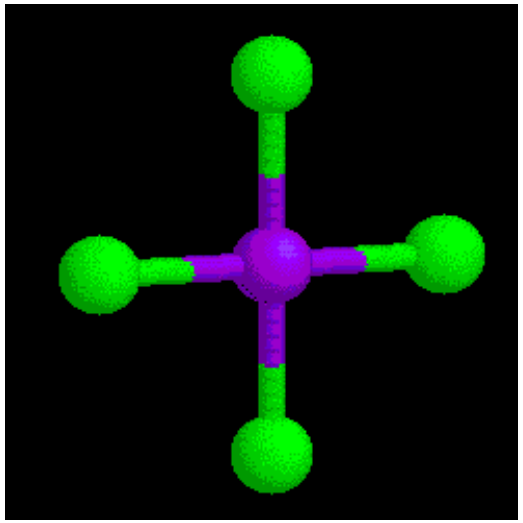
6 e^- pairs on central atom



6 shared, 0 unshared



5 shared, 1 unshared



4 shared, 2 unshared

Exercises

Write the Lewis structure and predict the molecular geometry of the following using VSPER Model. Draw in 3D.

1) OF_2
2) PF_3
3) XeF_6
4) SF_4
5) XeF_4
6) PH_3
7) SO_3

Molecular Geometry
Dipole Moment and Polarity

Polar bonds: electronegativity difference between atoms is >0.4.

Ex: H_2O

O(3.5) – H (2.1) = 1.4
Polar covalent bond

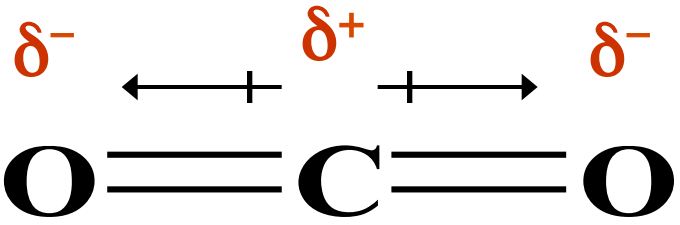
Polarity of Bonds

- Based on difference in electronegativity values
- 0.0- 0.4 nonpolar
- 0.4- 1.0 moderately polar covalent
- 1.0- 2.0 polar covalent
- ≥2.0 ionic

Polar bonds vs. Polar molecule

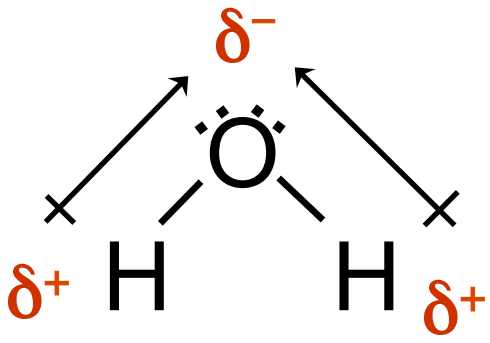
- Not all molecules with polar bonds are polar.
- It depends on the symmetry of the molecule
- Electrons will be pulled toward the most electronegative element in the bond.
- Different elements will pull electrons proportional to their electronegativity values.
- If electrons are evenly distributed, then the molecule is nonpolar.

Molecular Geometry
Dipole Moment and Polarity



nonpolar, bp=-79°C

dipole moment, μ = 0 D



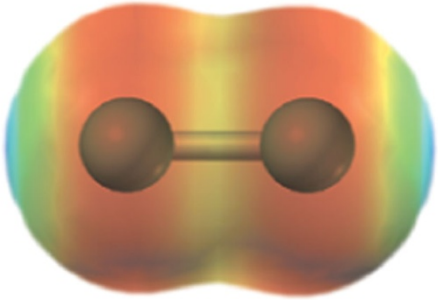
Net dipole

polar, bp=100°C

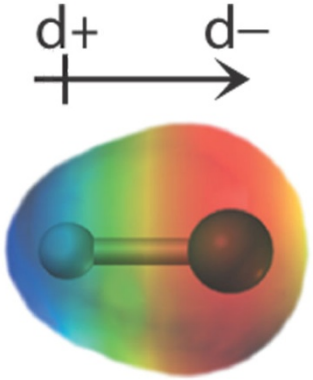
dipole moment, μ = 1.85 D

Dipole Moment and Molecular Geometry

Molecules that exhibit **any asymmetry** in the distribution of electrons would have a nonzero net dipole moment. These molecules are considered **polar**.

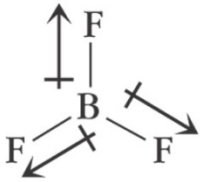


Non polar
VSEPR shape
identical atoms

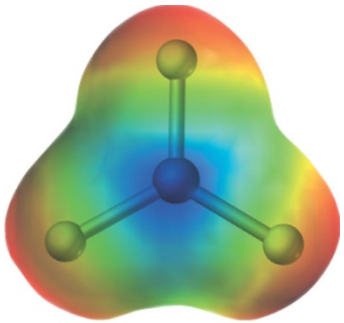


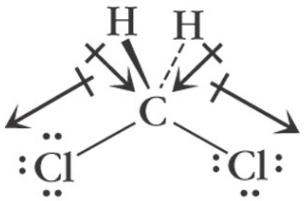
Polar
VSEPR shape
atoms differ

Dipole Moment and Molecular Geometry

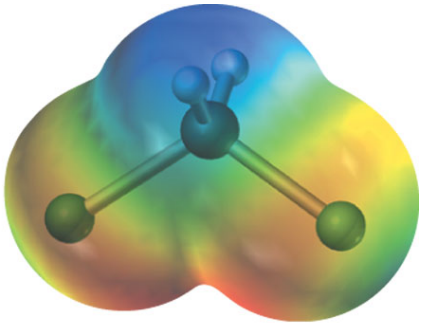


Bond dipoles cancel; no net dipole

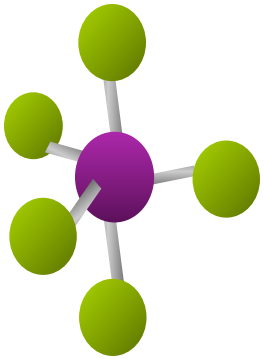




Net dipole



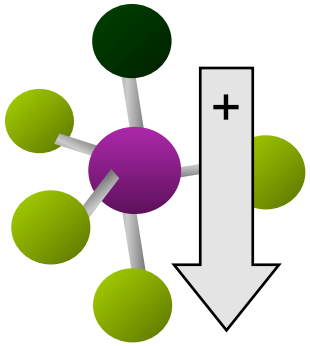
Molecular Geometry
Dipole Moment and Polarity



PF_5

Non polar

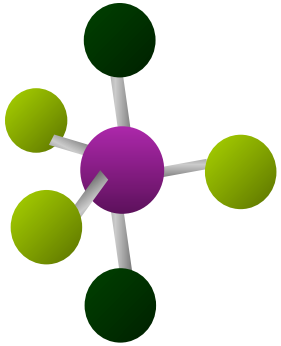
VSEPR shape
identical atoms



PF_4Cl

Polar

VSEPR
shape
atoms differ

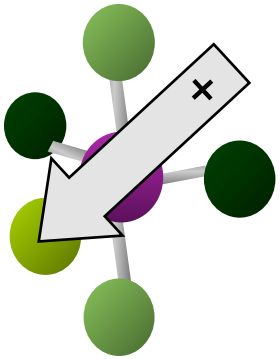


PF_3Cl_2

Non polar

Atoms differ. ***BUT*** can be divided into nonpolar VSEPR shapes:

linear + triangular planar



PF_3Cl_2

Polar

Atoms differ.
Doesn't divide into nonpolar VSEPR shapes

Polar vs. Nonpolar

- Go back to molecules from earlier slide and determine if they are polar or nonpolar.