VSEPR Rules

1. Draw the Lewis structure for the molecule or ion.

2. Count the total number of regions of electron density (bonding and lone electron pairs) around the central atom.

- Double and triple bonds count as *ONE REGION OF HIGH ELECTRON DENSITY.*
- An unpaired electron counts as *ONE REGION OF HIGH ELECTRON DENSITY.*

For molecules or ions that have resonance structures, you may use any one of the resonance structures.

3. Identify the most stable arrangement of the regions of electron density as *ONE* of the following:

- linear
- trigonal planar
- tetrahedral
- trigonal bipyramid
- octahedral

4. Determine the positions of the atoms based on the types of electron pairs present (i.e., bonding pairs vs. lone pairs).

The most stable configuration results when the electron pairs move into positions that minimize repulsion in order of:

lp-lp > lp-bp > bp-bp

For trigonal bipyramid and octahedral arrangements, there can sometimes be more than one possible arrangement of the bonding and lone pairs:

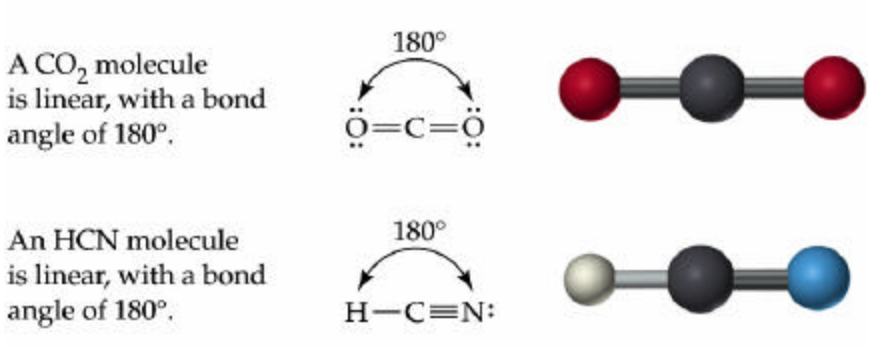
- Trigonal bipyramid - place any lone pairs in the plane of the triangle (Equatorial positions).
- Octahedral - if you have two lone pairs, place them on opposite sides of the central atom.

5. Identify the molecular geometry (**MG**) based on the positions of the *atoms* (NOT on the regions of high electron density).

6. Identify the electronic pair geometry (**EPG**) based on the positions of the *electron pairs*

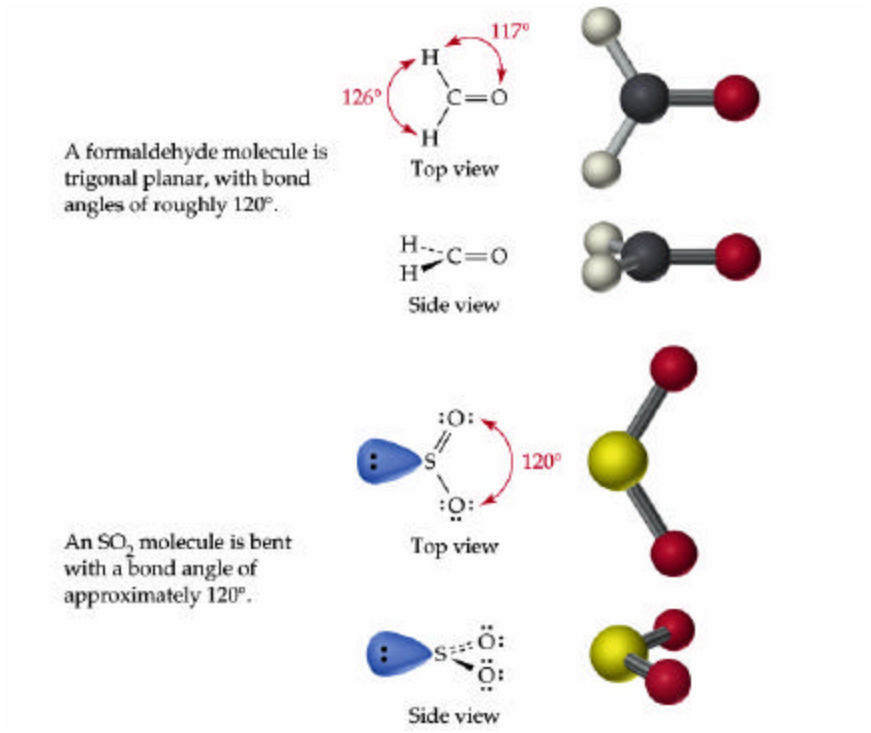
Linear Molecules

All diatomic and triatomic molecules with no loan pairs on the central atoms form a linear ***Molecular (MG) and Electron Pair Geometry (EPG)***



MG = Linear
EPG = Linear

Trigonal Planar and Bent Molecules

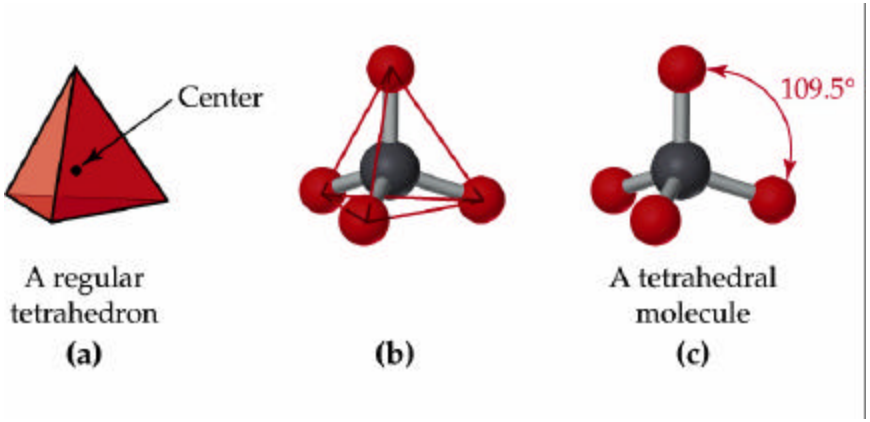


For a central atom bonding 3 atoms with no lone pairs, the MG = EPG = ***Trigonal Planar***.

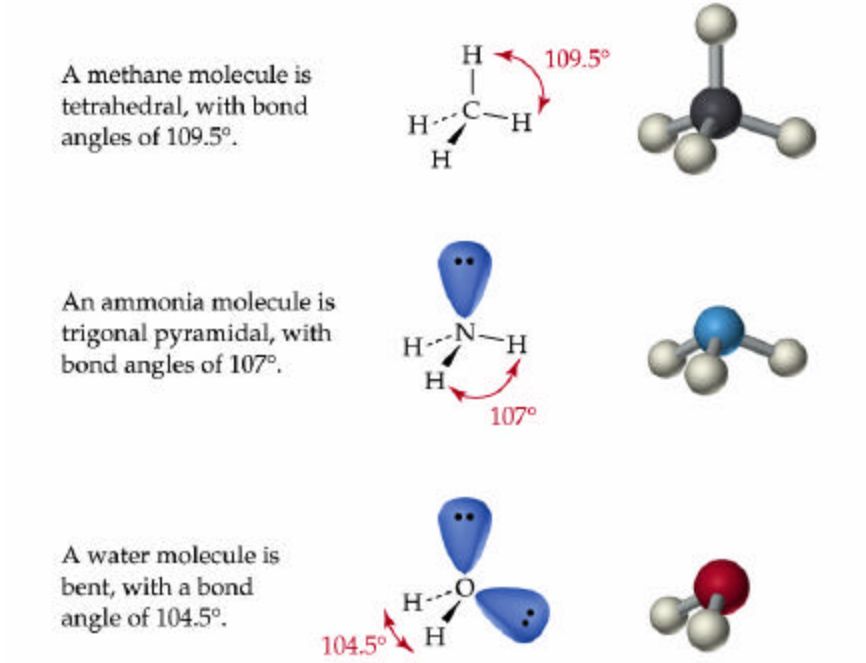
For a central atom bonding 2 atoms with 1 or 2 lone pairs, the MG = Bent and the EPG = trigonal planar.

Tetrahedral EPG

When a central atom has 4 regions of electron density (lp & bp) the EPG is defined by a ***Tetrahedron***.



Examples are:



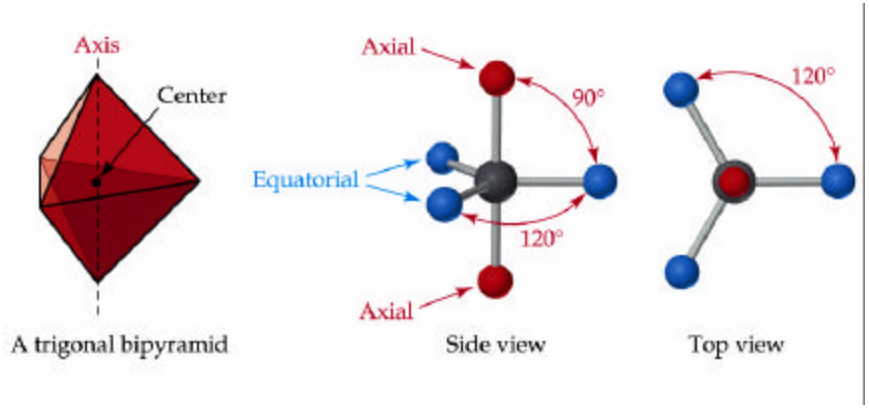
A central atom with 4 bonds has a MG = tetrahedral and an EPG = tetrahedral.

When there are 3 bonds and one lone pair as in ammonia (NH_3), the structure has a MG = trigonal pyramid while retaining the EPG = tetrahedral. The lone pair pushes the bonding pairs down out of the molecular plane to form the trigonal pyramid geometry.

In the case of water (H_2O) the two lone pairs force the molecule to bend into an angle. The MG = bent while the 4 electron pairs maintain a EPG = tetrahedral.

Expanded Valences

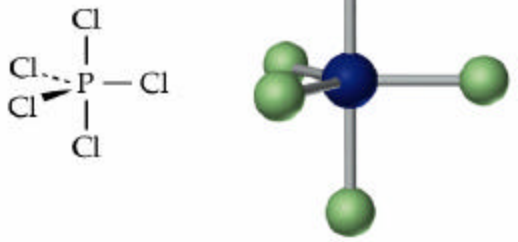
When a central atom is surrounded by 5 electron pairs, as is the case for an expanded valence, a ***Trigonal Bipyramid*** always describes the EPG.



PCl_5 is an example of an expanded valence compound that has a trigonal bipyramid MG and EPG.

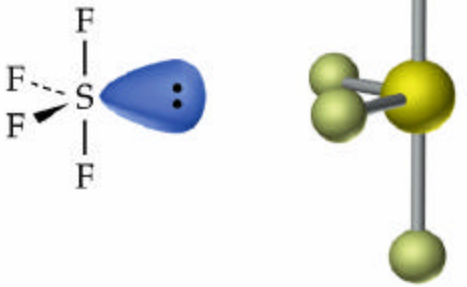
Since phosphorous is in the 3rd period, the 5 valence electrons can provide bonding for up to 5 atoms as seen to the right.

A PCl_5 molecule is trigonal bipyramidal.



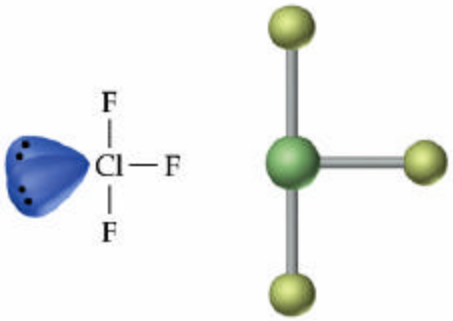
In the case of SF_4, the lone pair resides in an equatorial position creating a "See Saw" molecular geometry for the structure.
This is the lowest energy conformation since there are two 90° lp-bp interactions and two 120° lp-bp interactions. In the axial position, there would be three 90° interactions. This would result in a higher energy (less favorable) conformation.
The EPG remains trigonal bipyramid as there are 5 total regions of electron density.

An SF_4 molecule is shaped like a see-saw (turn 90° to see it).



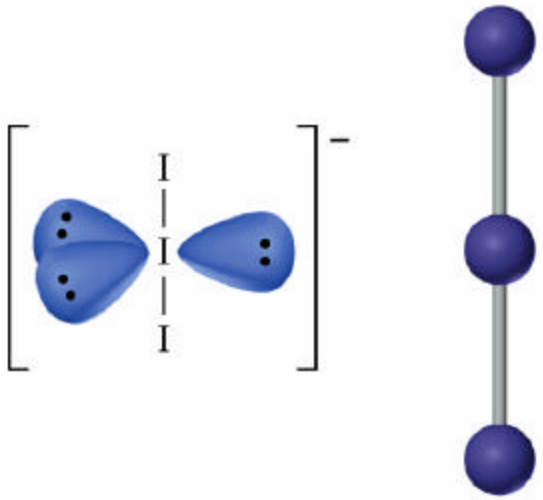
When a molecule has 5 electron pairs, 2 of which are lone pairs, the lone pairs reside in the equatorial positions forcing the bonding atoms into a "***T-Shaped***" molecular geometry.

A ClF_3 molecule is T-shaped (turn 90° to see it).



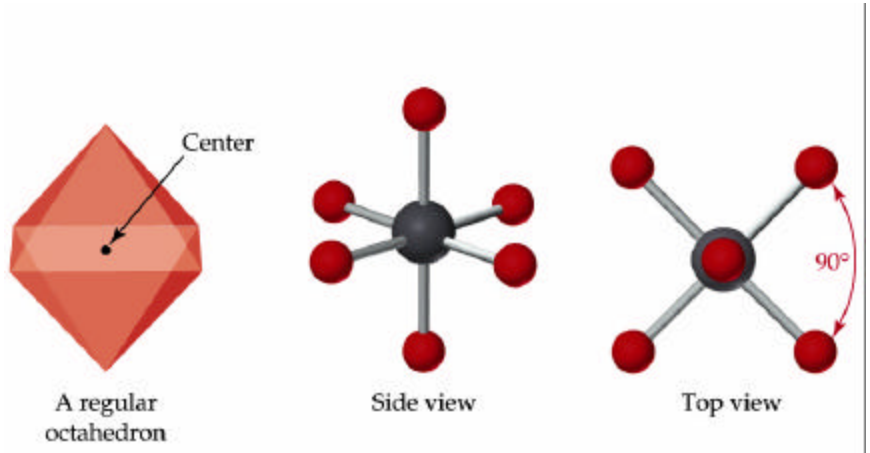
When a molecule that has a trigonal bipyramid EPG contains 2 bonds and 3 lp, the lp will occupy the equatorial positions to form the lowest energy confirmation. The result as in I_3^- is a linear molecular geometry (MG) with both I-I bonds in the axial positions.

An I_3^- ion is linear.



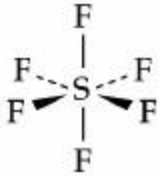
Some expanded valence compounds will have a total of 6 electron pairs (bp & lp) around a central atom.

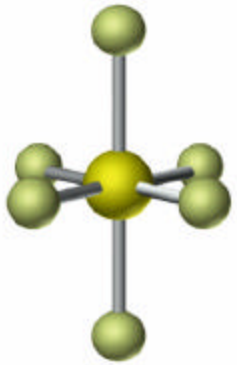
In this case, the EPG is described by a "octahedron" and EPG is called ***Octahedral***.



In SF_6, each of the 6 valence electrons in sulfur expands to form a bond with a F-atom. This results in a octahedral MG and EPG for the molecule.

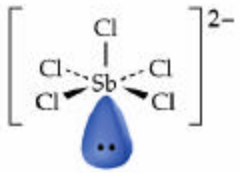
An SF_6 molecule is octahedral.

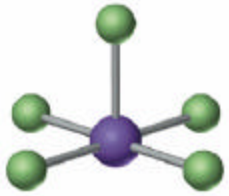




When an octahedral EPG contains 5 bonds and 1 lp, the lp will occupy and of the 6 positions as all are equivalent. The result is a molecular geometry that is described by a square pyramid. (like in Egypt) The MG is then called "***Square Pyramidal***".

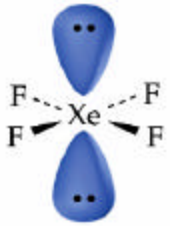
An $SbCl_5^{2-}$ ion has a square pyramidal shape.

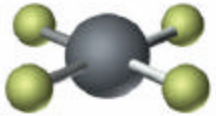




When an octahedral EPG has 4 bonds and 2 lp, the two lp will occupy positions opposite of one another to form the most stable conformation. The result is a "***Square Planar***" MG as in XeF_4.

An XeF_4 molecule has a square planar shape.





The following tables summarize the examples of each VESPR case listed. For more information please consult your text, the library and of course, the web!

All figures courtesy of "Chemistry", John McMurry & Robert C. Fay 3rd edition, Prentice Hall Publications.

TABLE 7.4 Molecular Geometry Around Atoms with 2, 3, 4, 5, and 6 Charge Clouds

Number of Bonds	Number of Lone Pairs	Number of Charge Clouds	Molecular Geometry	Example
2	0	2	Linear	O=C=O
3	0	3	Trigonal planar	H–C(=O)–H
2	1		Bent	O–S–O
4	0	4	Tetrahedral	CH4
3	1		Trigonal pyramidal	NH3
2	2		Bent	H2O

Continued

TABLE 7.4 (Continued)

Number of Bonds	Number of Lone Pairs	Number of Charge Clouds	Molecular Geometry	Example
5	0	5	Trigonal bipyramidal	PCl5
4	1		See-saw	SF4
3	2		T-shaped	ClF3
2	3		Linear	I3–
6	0	6	Octahedral	SF6
5	1		Square pyramidal	SbCl5 2–
4	2		Square planar	XeF4