Valence Shell Electron Pair Repulsion Theory

VSEPR theory is used to predict the shape of molecules. Shape can be important for polarity, solubility, boiling points and ability to chemically react.

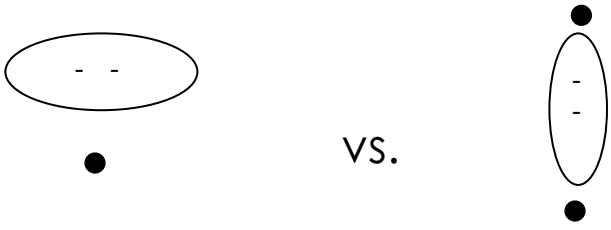
1. The valence bonded or unbonded pairs of e- are viewed as –ve charge clouds.

2. These clouds repel each other.

3. To achieve minimum potential energy it is necessary to locate these clouds as far away from each other as possible.

4. Since the clouds are associated with atoms, once the clouds are located the atoms can be located thereby determining shape of molecule

5. Unbonded pairs occupy more volume than bonded pairs.



Causes angles to be smaller

6. VSEPR applies to the geometry around the central atom.

***AXE Method** of electron counting is commonly used when applying the VSEPR theory.*

The *A* represents the central atom and always has an implied subscript one.

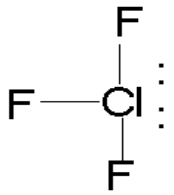
The *X* represents the number of sigma bonds between the central atoms and outside atoms. Multiple covalent bonds (double, triple, etc) count as one *X*.

The *E* represents the number of lone electron *pairs* (unbonded) surrounding the central atom.

The geometry of the molecule is also associated with the total number of hybridized orbitals used by valence bond theory.

VSEPR CODE: AX_3E_2

ex. ClF_3



Based on distribution of *X*'s and *E*'s, VSEPR theory makes the predictions in the following tables. Note that the geometries are named according to the atomic positions only and not the electron arrangement. For example, even though AX_2E_1 and AX_2 are both bent molecules the actual angles may be different due the number of lone pairs on the central atom.

RULES FOR FINDING LONE PAIRS OF ELECTRONS

1. Add up all of the valence electrons (remember to include any charges) Eg. NCl_3 → 5 + (3*7) = 26e
2. Subtract 8 electrons for every outer atom (only 2 for Hydrogen). The difference divided by 2 gives the number of lone pairs

Eg. 3*8 = 24e on outer Cl's

total e = 26
-24
2

Divide that difference by two to get the number of lone pairs
ie) 2/2 =1
There is one lone pair on the N.

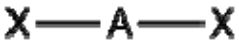
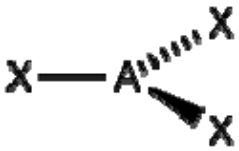
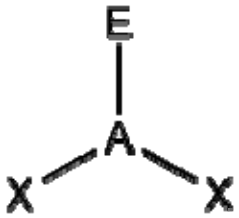
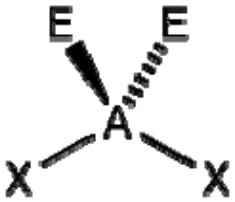
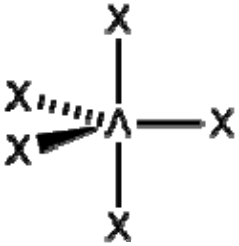
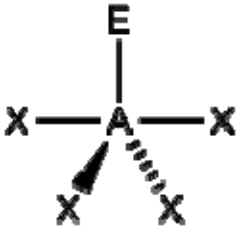
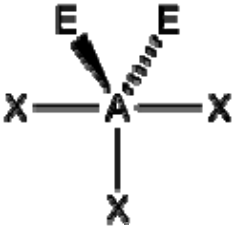
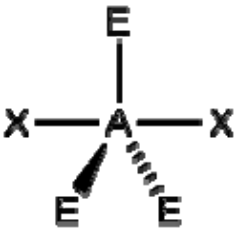
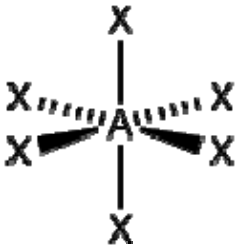
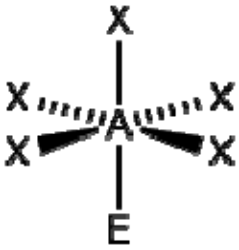
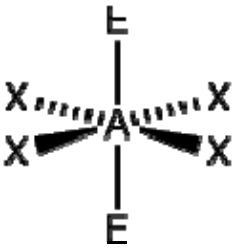
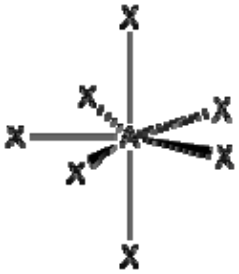
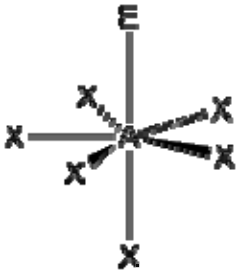
Therefore the basic shape → <u>3 bonding pairs + 1 lone pair</u>
= 4 pairs → tetrahedral.

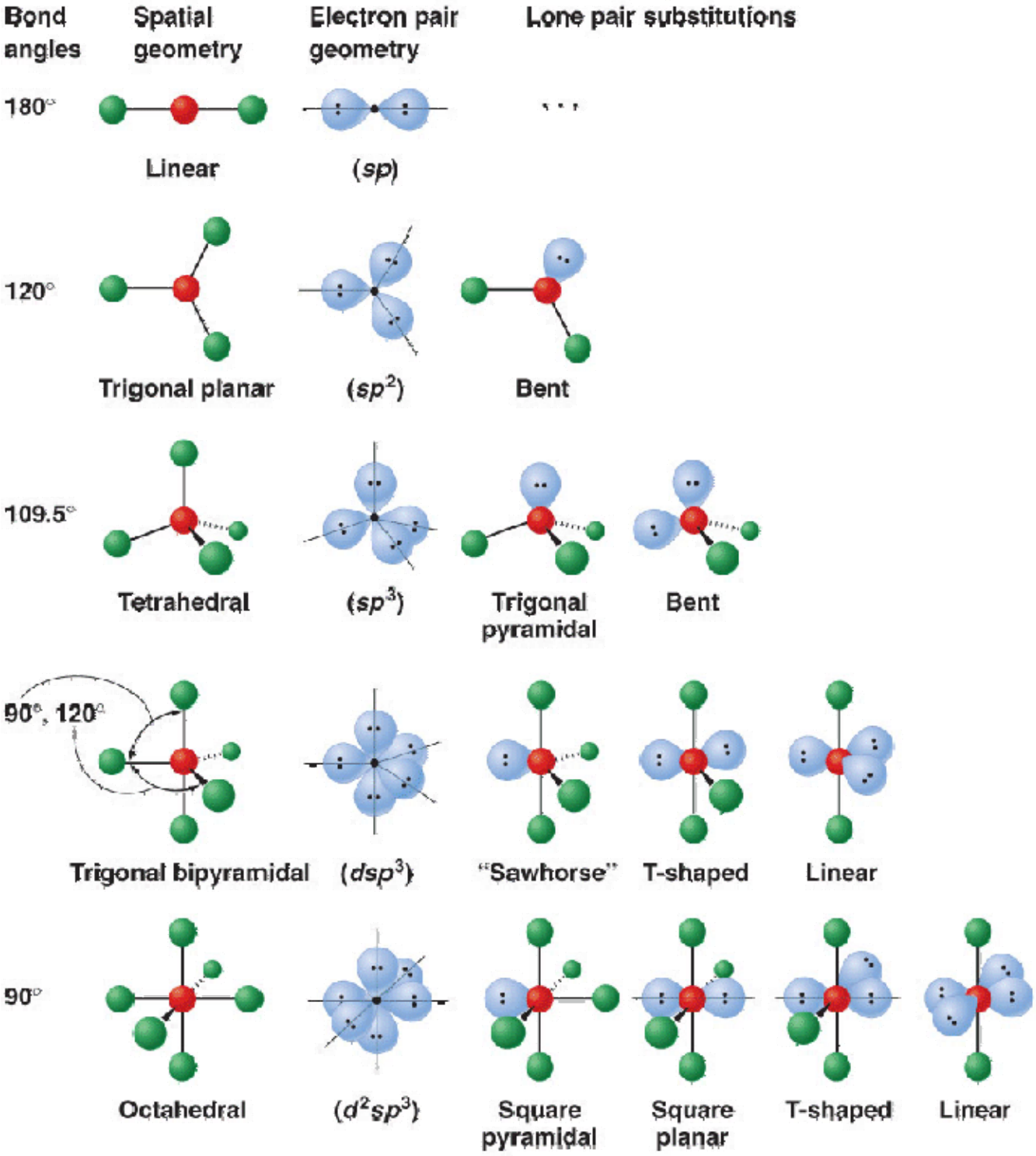
- Actual shape, since one of those pairs has no atom on it is ***<u>trigonal pyramid.</u>***

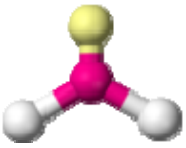
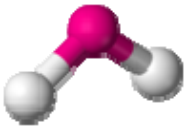
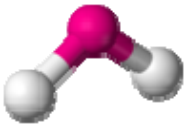
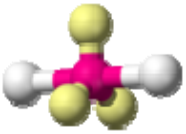
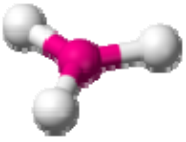
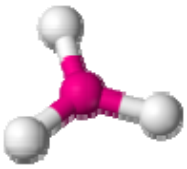
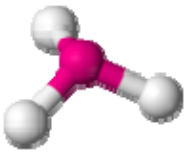
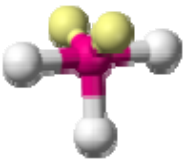
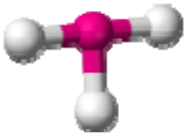
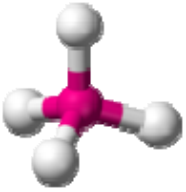
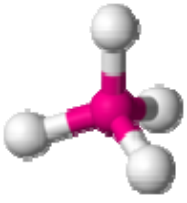
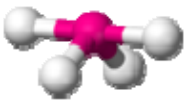
Do the following examples:

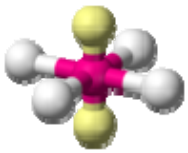
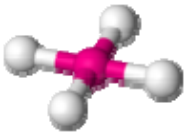
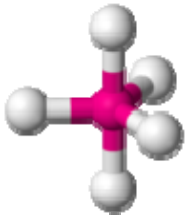
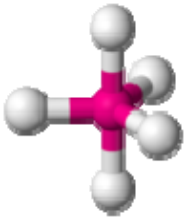
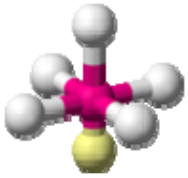
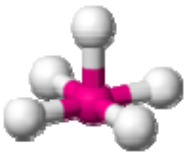
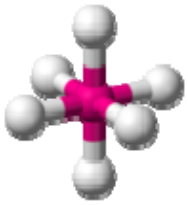
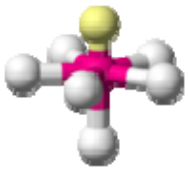
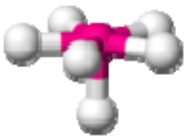
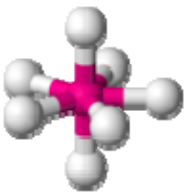
HCl BF_3 H_2O NH_3 PCl_5 CH_4 $HCCl_3$

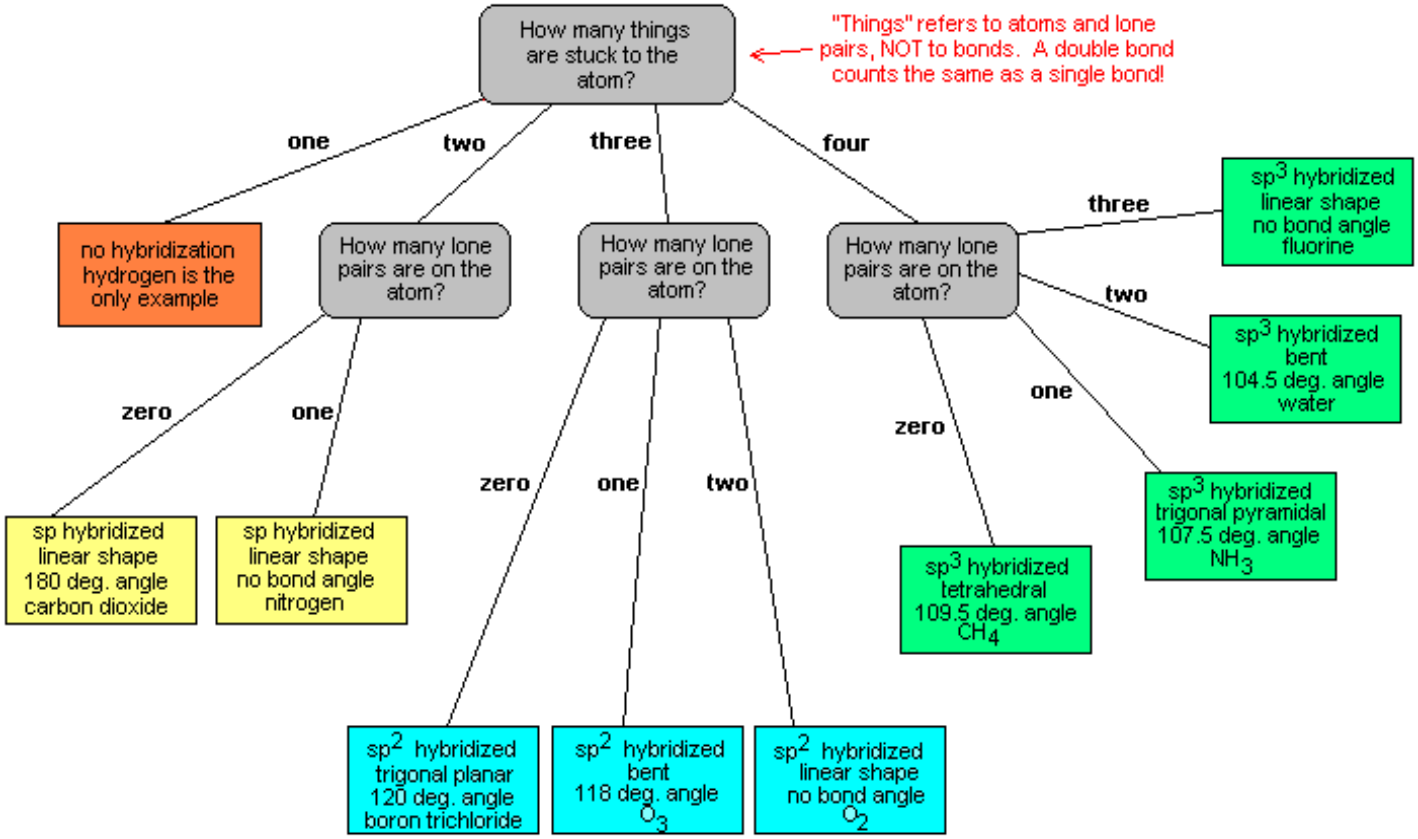
NH_4^+ CO_3^{-2} NH_2^- CO_2

Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs
2	 Linear			
3	 Trigonal planar	 Bent		
4	 Tetrahedral	 Trigonal pyramid	 Bent	
5	 Trigonal bipyramid	 Seesaw	 T-shaped	 Linear
6	 Octahedral	 Square pyramid	 Square planar	
7	 Pentagonal bipyramid	 Pentagonal pyramid		



Molecule Type	Shape	Electron arrangement†	Geometry‡	Examples
AX_1E_n	Diatomic			HF, O_2
AX_2E_0	Linear			$BeCl_2$, $HgCl_2$, CO_2
AX_2E_1	Bent			NO_2^-, SO_2, O_3
AX_2E_2	Bent			H_2O, OF_2
AX_2E_3	Linear			XeF_2, I_3^-
AX_3E_0	Trigonal planar			BF_3, CO_3^{2-}, NO_3^-, SO_3
AX_3E_1	Trigonal pyramidal			NH_3, PCl_3
AX_3E_2	T-shaped			ClF_3, BrF_3
AX_4E_0	Tetrahedral			CH_4, PO_4^{3-}, SO_4^{2-}, ClO_4^-
AX_4E_1	Seesaw			SF_4

AX_4E_2	Square planar			XeF_4
AX_5E_0	Trigonal bipyramidal			PCl_5
AX_5E_1	Square pyramidal			ClF_5, BrF_5
AX_6E_0	Octahedral			SF_6
AX_6E_1	Pentagonal pyramidal			$XeOF_5^-$, IOF_5^{2-} [7]
AX_7E_0	Pentagonal bipyramidal			IF_7



1) Draw the Lewis structure for the molecule. This vital if you're going to get the answer right.

2) Count the number of "things" on the atom you're interested in. Let's say that you're looking at methane, CH_4. If you want to find the bond angles, shape, and hybridization for carbon, count the number of things that are stuck to it.

Now, the vague term "things" refers to atoms and lone pairs. IT DOES NOT REFER TO THE NUMBER OF BONDS! When you look at methane, there are four atoms stuck to it, so you'd go down the line that says "four" toward the green boxes on this chart.

People get confused with multiple bonds. Take carbon dioxide, for example. There are four bonds (carbon is double-bonded to each oxygen) but only two oxygen atoms bonded to carbon. In this case, we count two things stuck to carbon, because we only count the atoms, NOT the number of bonds.

Likewise, with ammonia there are four things. Three of the things on nitrogen are hydrogen atoms and the fourth is a lone pair. For the purposes of VSEPR, lone pairs count exactly the same as atoms, because they consist of negative charge, too.

3) Count the number of lone pairs that are on the atom you're interested in. IMPORTANT: This does NOT mean to count the number of lone pairs on all of the atoms in the molecule. Lone pairs on other atoms aren't important - what's important is only what's directly stuck to the atom you're interested in.

We mentioned above that methane has four things stuck to it. Since all four things are hydrogen atoms, we moved toward the green boxes on the flow chart. When we get to our second question, we find that there are no lone pairs on carbon, so our answer is zero. When we go down the line that says "zero" from that box, we find that methane is sp^3 hybridized, with a 109.5 degree bond angle and tetrahedral shape.

And, hey, that's what we were looking for!