

VSEPR

Valence Shell Electron Pair Repulsion Theory

This theory helps us to predict the SHAPE of a molecule. To do so, all you have to do is follow 5 rules (memorize them!).

1

RULES FOR VSEPR

1. Determine the CENTRAL atom and its number of valence electrons.

2. For EACH hydrogen or halogen attached, add 1 to the total above.

3. If you have an ion: For each + charge, subtract 1 from the total thus far. For each - charge, add 1 to the total thus far.

2

4. Divide the total by 2 to get the number of electron pairs. Arrange the pairs around the central atom so that they are as far apart from one another as possible. (This is called the electron pair ARRANGEMENT.)

5. Attach the atoms (to the central one) to determine the final molecular SHAPE.

3

CO₂

1. The central atom is carbon and it has 4 valence e⁻.

2. It has no halogens attached nor hydrogen.

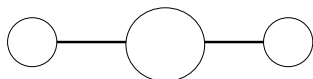
3. It is not an ion.

4. Four divided by 2 = 2 electron pairs.

5. With carbon in the middle, one oxygen on each side will make a LINEAR shape like this:

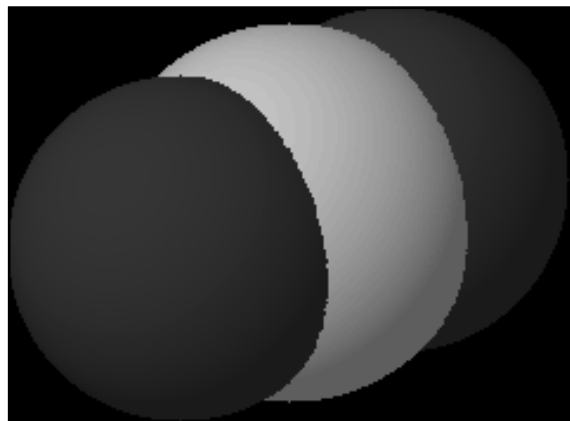
4

Linear

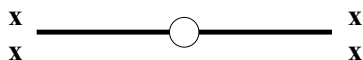


Note that the bond angles between the central atom and each of the attached atoms is obviously 180°.

5

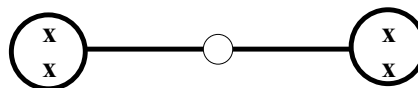


How do you DRAW a linear arrangement of electron pairs?



7

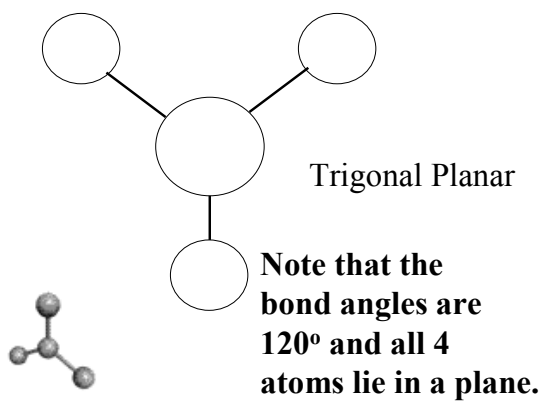
How do you DRAW a linear shape?



8

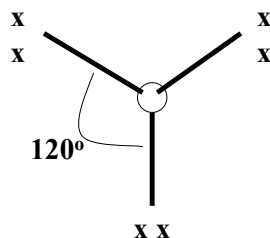
BF₃?

1. The central atom is boron which has 3 valence e⁻.
2. There are 3 halogens attached so add 3 (=6).
3. It is not an ion.
4. 6 divided by 2 = 3 electrons pairs.
5. When all 3 atoms are attached to the boron, you will have a **TRIGONAL PLANAR** shape like this:



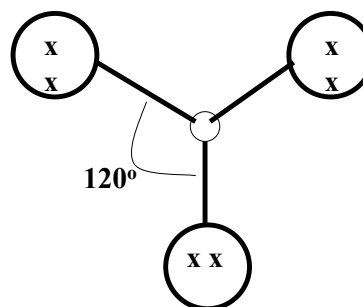
10

How do you DRAW a trigonal planar arrangement of electron pairs?



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How do you DRAW a trigonal planar shape?

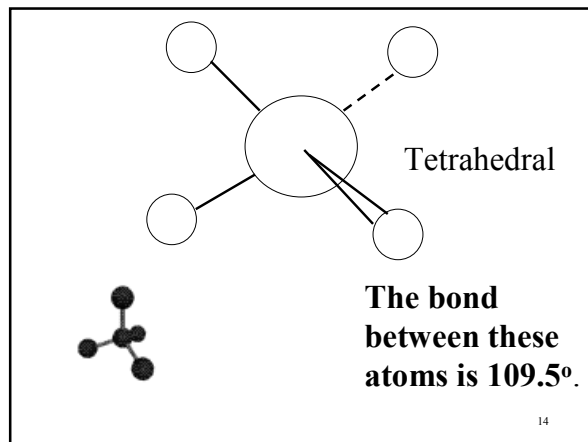


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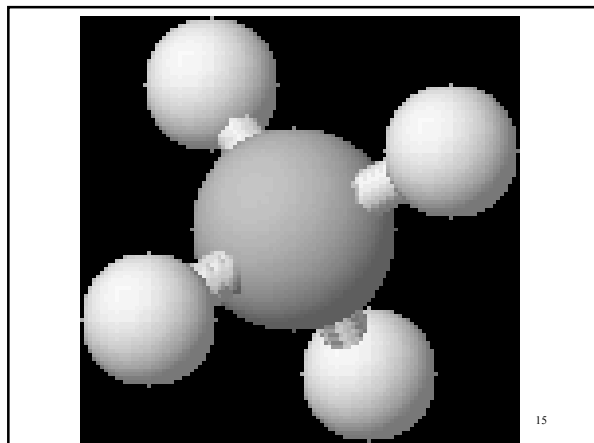
Methane, CH₄

1. Carbon is the central atom which has 4 valence e⁻.
2. There are 4 hydrogen atoms attached so add 4 more.
3. Methane is not an ion.
4. 8 divided by 2 = 4 electron pairs.
5. When you attach the 4 hydrogens to the carbon, you get a **TETRAHEDRAL** shape like this:

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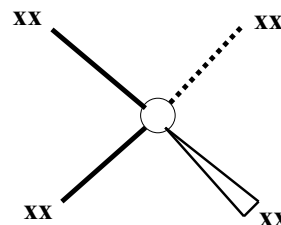


14



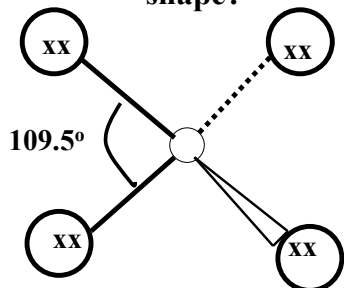
15

How do you DRAW a tetrahedral arrangement of electron pairs?



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How do you DRAW a tetrahedral shape?




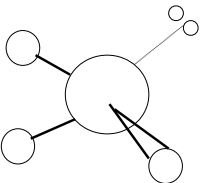
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Ammonia, NH₃

1. Nitrogen is the central atom which has 5 valence e⁻.
2. There are 3 hydrogens attached so add 3 (=8).
3. Ammonia is not an ion.
4. 8 divided by 2 = 4 electron pairs.
5. When you attach the 3 hydrogens to the nitrogen, you see that you have one non-bonding electron pair on the nitrogen and make a **TRIGONAL PYRAMIDAL** shape.

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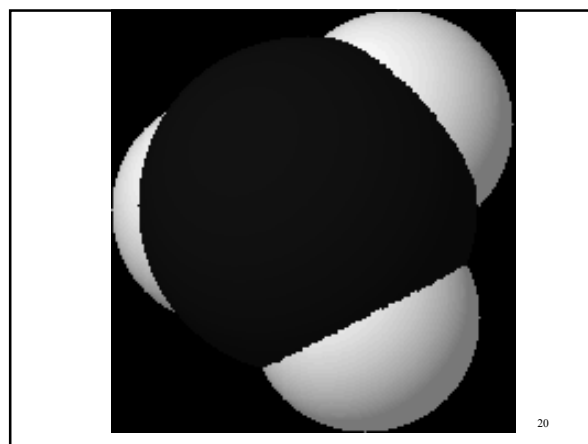
Trigonal pyramidal

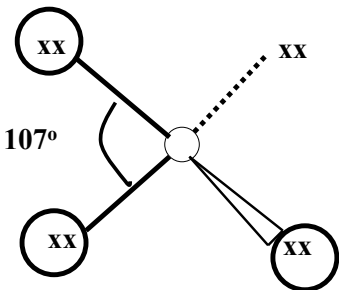
The bond angles here are *less than* the 109.5° of the tetrahedral angle due to electron repulsion -- they are $\sim 107^\circ$.

Note: You START OUT with a tetrahedral ARRANGEMENT of electron pairs!

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How do you DRAW a trigonal pyramidal shape?



107°


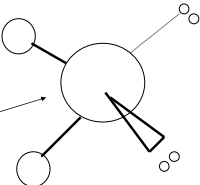
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Water: H_2O

- Oxygen is the central atom with 6 valence e^- .
- There are 2 hydrogens attached (=8).
- Water is not an ion.
- 8 divided by 2 = 4 electron pairs.
- When you add the two hydrogens to the oxygen atom, notice that oxygen will have 2 non-bonding pairs of electrons. You start out with a tetrahedral ARRANGEMENT of electrons but the final shape of the molecule is ANGULAR or BENT.

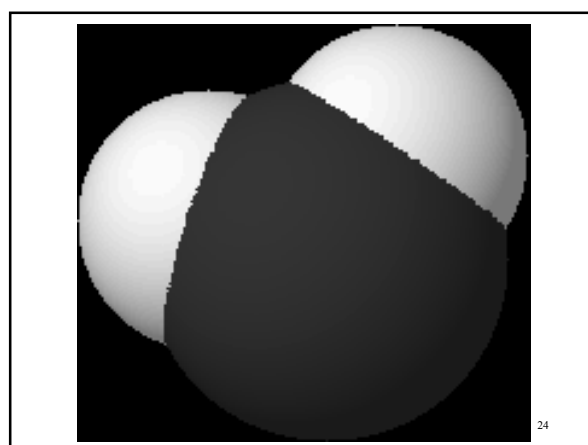
22

Angular or bent

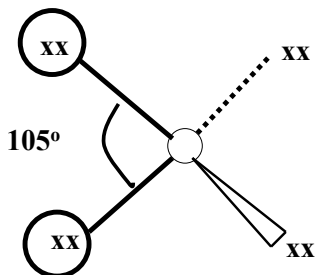



The bond angles here are $\sim 105^\circ$.

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How do you DRAW an angular shape?

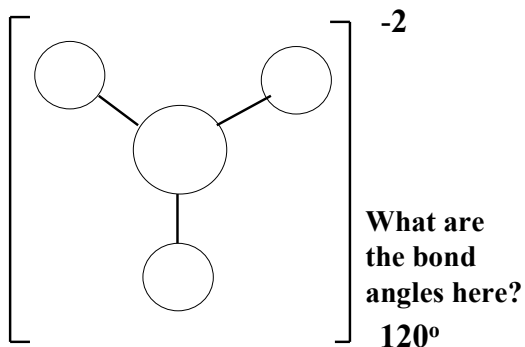


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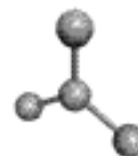
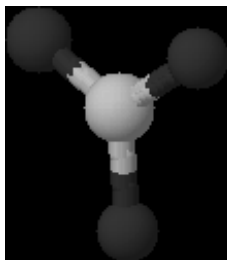


1. Carbon is the central atom which has 4 valence e^- .
2. There are no hydrogens nor halogens attached.
3. This ion has a -2 charge so add 2 (=6).
4. 6 divided by 2 = 3 pair of electrons.
5. When the carbon has the 3 oxygens attached, you get a TRIGONAL PLANAR shape.

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For each of the following, use VSEPR to determine the molecular shapes:

CS_2	Linear
BeBr_2	Linear
OCl_2	Angular/Bent
SF_2	Angular/Bent
H_3O^{+1}	Trigonal pyramidal
SiH_4	Tetrahedral

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Now for the cooler shapes....We can get some very interesting shapes for some molecules but don't try to do the Lewis structures for them (it won't work).

For a molecule of PCl_5

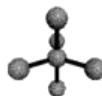
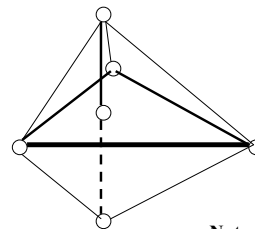
30



1. The central atom is phosphorus which has 5 valence e^- .
2. There are 5 halogens attached (=10).
3. This is not an ion.
4. 10 divided by 2 = 5 pair.
5. When you attach the atoms (no non-bonding electron pairs), you get a **TRIGONAL BIPYRAMIDAL** shape.

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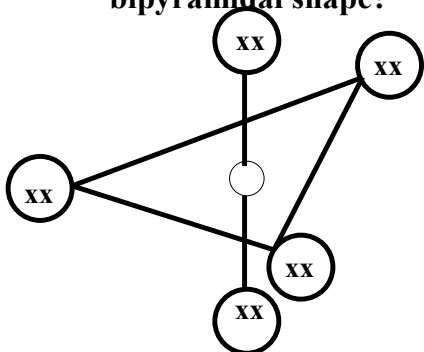
Trigonal bipyramidal



Note that the triangle must be drawn "at a slant" but the 3 points are all equidistant from the center.

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How do you DRAW a trigonal bipyramidal shape?



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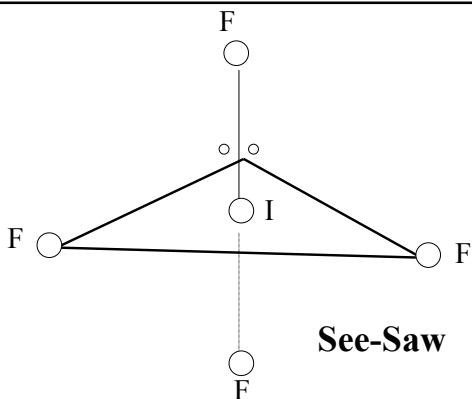


VSEPR = 5 electron pairs

Trigonal bipyramidal arrangement of electron pairs.

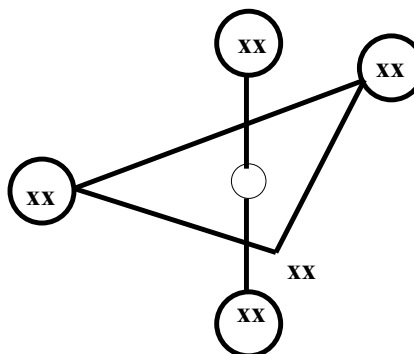
BUT, only 4 fluorine atoms attached and one non-bonding electron pair....

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How do you DRAW a see-saw shape?



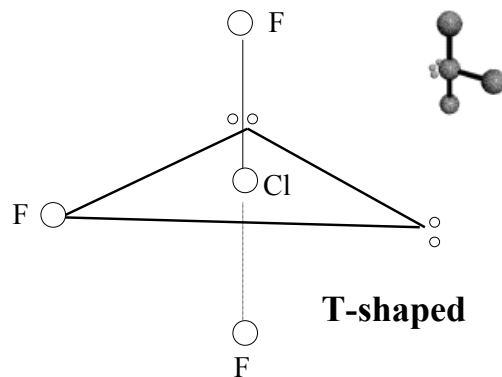
36

ClF_3 that's *chlorine*

VSEPR = 5 electron pairs so trigonal bipyramidal arrangement of electrons.

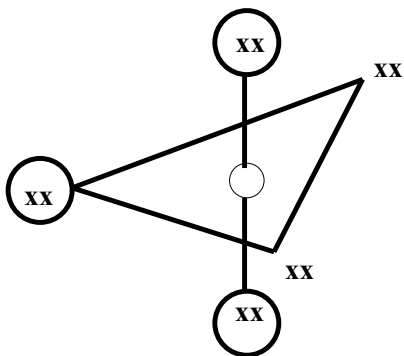
Attaching 3 fluorine atoms will leave you with 2 non-bonding electron pairs.

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How do you DRAW a T-shape?



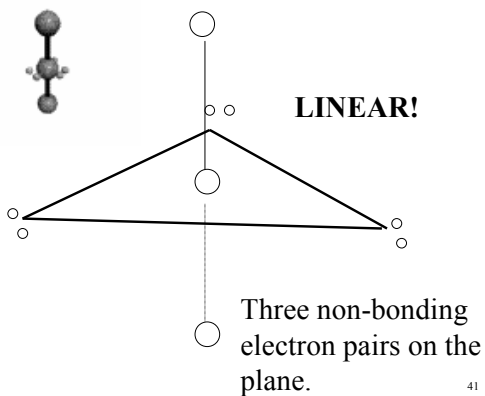
39

I_3^{-1} ?

VSEPR arithmetic = 5 electron pairs
Therefore, electron pair arrangement is trigonal bipyramidal.

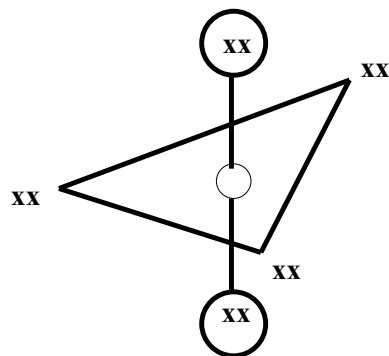
However, note that there are only two iodine atoms attached. They want to be as far apart as possible. Where would they be? Where would the 3 pair of non-bonding electrons be?

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How do you DRAW a linear shape?



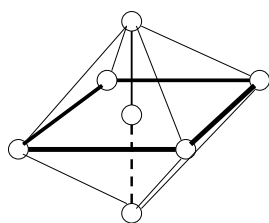
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Let's do OF_6

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1. Oxygen is the central atom which has 6 valence e^- .
2. There are 6 halogens attached (=12).
3. This molecule is not an ion.
4. 12 divided by 2 = 6 electron pairs.
5. When you attach the 6 fluorine atoms around the oxygen (and getting them as far apart from one another as possible), you will have an **OCTAHEDRAL** shape.

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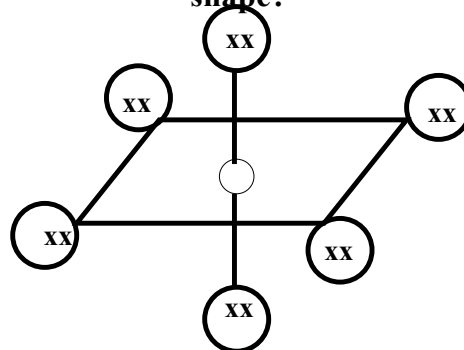
Octahedron



Can you see that if you drew lines from each equidistant point that you would have an 8 sided figure (hence the name!)?

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How do you **DRAW** an octahedral shape?

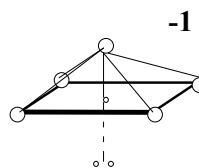


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OBr_5^{-1} ?

1. Oxygen is the central atom and has 6 valence e^- .
2. There are 5 halogens attached (=11).
3. Since this ion has a -1 charge, add 1 (=12).
4. 12 divided by 2 = 6 pair of electrons.
5. You start out with an octahedral **ARRANGEMENT** of electrons but since there are only 5 bromine atoms attached, you will have a **SQUARE PYRAMIDAL** shape.

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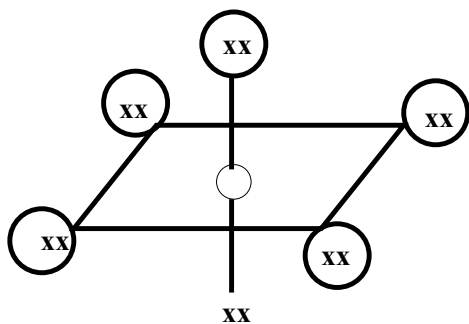
Square pyramidal



The red lines here help you to visualize this shape.

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How do you DRAW a square pyramid?



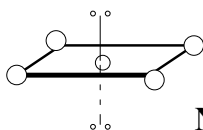
49



1. Xenon is the central atom and has 8 valence e⁻.
2. There are 4 halogens attached (=12).
3. This molecule is not an ion.
4. 12 divided by 2 = 6 electron pairs.
5. While you start out with an octahedral ARRANGEMENT of electron pairs, since there are only 4 fluorine atoms attached, you will have a **SQUARE PLANAR** molecule shape.

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Square Planar

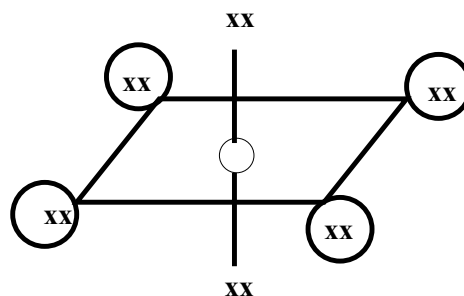


Notice that in this shape, you have 2 non-bonding electron pairs.



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How do you DRAW square plane?

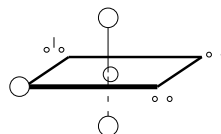


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- Xe is the central atom with 8 valence electrons.
- There are 3 halogens attached so $8 + 3 = 11$.
- It is an ion so ADD one (-1 charge) = 12.
- Divide by 2 so 6 electron pairs → octahedral arrangement of electron pairs.
- Attach the 3 chlorine atoms. What shape do you have?

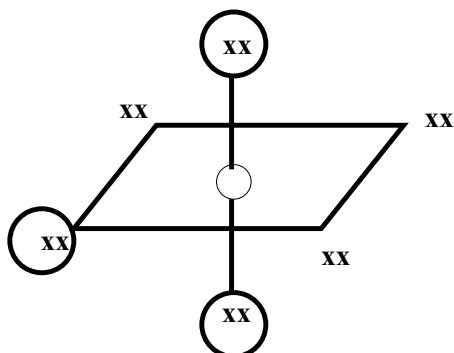
53



This is called a T-shape.

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How do you DRAW T-shape?



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Try these on your own now:

SO_2
 AsCl_3
 SF_2
 XeOF_4 (Xe is the central atom)
 AsF_5
 ICl_4^{-1}
 XeO_4
 O_3
 Br_3^{-1}

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ANSWERS:

SO_2	Angular or bent
AsCl_3	Trigonal pyramidal
SF_2	Angular or bent
XeOF_4	Square pyramidal
AsF_5	Trigonal bipyramidal
ICl_4^{-1}	Square planar
XeO_4	Tetrahedral
O_3	Angular or bent
Br_3^{-1}	Linear

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In summary, follow the VSEPR rules.

ARRANGEMENT of electron pairs	Molecular SHAPES
1 pair	Linear
2 pair	Linear
3 pair	Trigonal planar
4 pair	Tetrahedral
5 pair	Trigonal bipyramidal
6 pair	Octahedral

Lines connect the shapes in the table to the following list of molecular shapes:

- Linear
- Angular or bent
- Trigonal planar
- Tetrahedral
- Trigonal pyramidal
- Bent
- Trigonal bipyramidal
- See-saw
- T-shaped
- Linear
- Octahedral
- Square pyramidal
- Square planar

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REMINDER!

1. The shape of a molecule is determined by the atoms attached to a central atom.
2. Non-bonding electron pairs influence the shape by repelling the attached atoms to some degree.
3. Keep in mind that when you are trying to figure out a molecular shape, the attached atoms want to be as far apart from one another as possible. And, you must arrange them in 3 dimensions!

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