Shapes of Molecules

All shapes came from

http://www.spusd.k12.ca.us/chemmybear/shapes.html

VSEPR theory

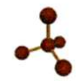
- Valence shell electron pair repulsion theory
- Simply stated it says- all atoms and electrons pairs will stay as far apart from one another as possible in 3-D space.
- This is because electrons and the electron shells of each atom are negative and therefore repel each other.
- We will only deal with the simple shapes around one *center* atom

So you have to imagine the shape we drew was in 3-D

So something like methane - CH_4

H
H -C- H
H

Really looks like this



This shape is called Tetrahedral

The bond angle is 109.5º

Now if you have an unbonded pair of electrons…

Something like ammonia NH_3

The electron pair still repels the atoms so it looks like…

..
H – N – H
H

This shape is called Trigonal Pyramidal

A tetrahedron without the top piece, or a triangle that is bent downwards

The bond angle is 109.5º

If you have 2 pairs of unbonded electrons

Something like water H_2O

You get a shape that looks like

..
:O – H
H

This shape is called Bent

A "V" shape

The bond angle is 109.5º

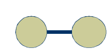
If you have 3 unbonded electron pairs

Something like Chlorine gas, Cl_2

.. ..
:Cl-Cl:
.. ..

It looks exactly like we draw it

This shape is called Linear



A straight line

Steric number

- Steric number- how many spots an atom has for pairs of electrons or bonds
- steric number = bonds + unshared electron pairs
- **Every atom so far had a steric number of 4**
- Steric number can go from 2-6
- Double/Triple bonds count as 1 bond.
- *only get the steric number for the **ONE** center atom

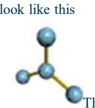
Steric number of 3

Like BF_3 or CH_2O

|F|
B-F|
|F|

H
C=O
H

Will look like this



This is called Trigonal Planar

A flat triangle

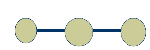
The bond angle is 120º

Steric number of 2

Like CO_2 carbon dioxide

O = C = O

Is again a linear shape
it looks exactly as it is drawn

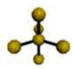


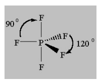
The bond angle is 180º

Steric number of 5

Like PF_5 Phosphorus pentafluoride

Would look like





This is called
Trigonal Bipyramidal

Steric # 5 with unbonded pairs of electrons

- With one pair of unbonded electrons it is a See-saw shape (SF_4, IOF_4)
- With two pairs of unbonded electrons it is T-Shaped (ClF_3, BrF_3)
- With 3 unbonded pairs of electrons it is linear (XeF_2)

Steric number of 6

Like SF_6 sulfur hexafluoride

*really electronegative elements can break the octet rule

Would look like

This shape is Octahedral

The bond angle is 90°

Steric # of 6 with unbonded pairs of electrons

- With one unbonded pair of electrons it is square pyramidal. ($XeOF_4$)
- With two unbonded pairs of electrons it is square planar. (XeF_4)

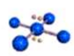
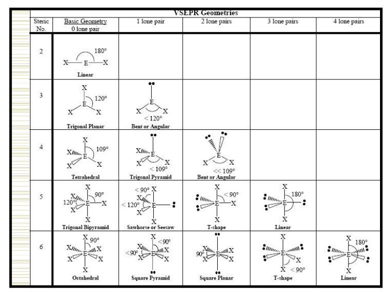


Table of all shapes

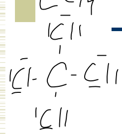
e^- pairs	Steric # 2	Steric # 3	Steric # 4	Steric # 5	Steric # 6
0	Linear	Trigonal planar	tetrahedral	Trigonal Bipyramidal	octahedral
1	(linear)	(bent)	trigonal pyramidal	Seesaw	Square pyramidal
2	n/a	(linear)	bent	T-Shaped	Square Planar
3	n/a	n/a	(linear)	Bent	T-Shaped



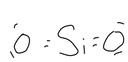
Examples

- Draw the Lewis Dot, predict the shape and bond angle for:
- CCl_4
- SiO_2
- $SiOF_2$
- SeF_6
- PF_5
- PCl_3
- NO_2^- (nitrite ion)

CCl_4 | SiO_2

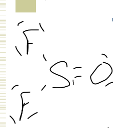


tetrahedral
109.5°

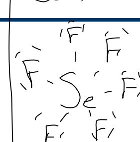


linear
180°

$SiOF_2$ | SeF_6

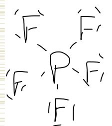


trigonal planar
120°

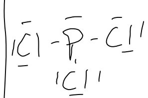


octahedral
90°

PF_5 | PCl_3

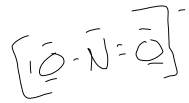


trigonal bipyramidal
90°/120°



trigonal pyramidal
109.5°

NO_2^-

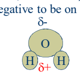


bent
120°

Molecular polarity vs. bond polarity

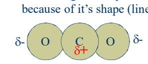
- Both water are CO_2 have polar bonds, however, only water is a polar molecule. CO_2 is nonpolar.

The shape of the water molecule (bent) allows the positive and negative to be on opposite sides



To be polar you need a positive end and a negative end

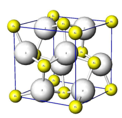
CO_2 is a nonpolar molecule even though it has polar bonds because of it's shape (linear)



Negative at both ends cancel out

Ionic shape

- Ionic compounds don't have a "shape", it is just an arrangement of positive and negative ions.



- Although a polyatomic ion can have a shape.