

Chemistry 6A Fall 2007

Dr. J. A. Mack

Monday

10/8/07

- Exams will be returned in your labs.
- Solutions are on the web.
- I will post grade summaries as soon as I get them from your lab instructors.
- No, the exam is not “curved”... Your score reflects your knowledge of the material thus far.
- If you did poorly, you need to consider your future status in this course.
- The material and skills learned in this course are critical for success in chem. 6B.

Molecular Shapes: Valence Shell Electron Pair Repulsion

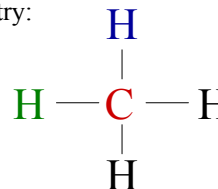
In order to predict molecular shape, we assume the valence electrons of each atom in the molecule repel one another.

When this occurs, the molecule adopts a 3D geometry that minimizes this repulsion where:

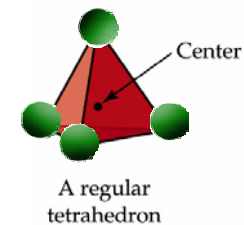
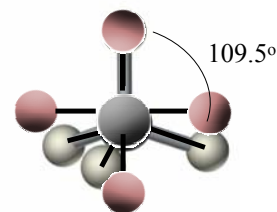
This process is known as:

Valence Shell Electron Pair Repulsion theory.
(VSEPR)

To accommodate the 109.5° bond angles, the atoms adopt a new 3-D geometry:



The H-atoms fit at the corners of a regular *tetrahedron* shape with the carbon at the center.



The molecular geometry of CH_4 is said to be “*tetrahedral*”

Drawing a Lewis structure in 3-D perspective:



The solid lines indicate that the bond is in the plane of the screen, the dashed indicates that the bond is behind the screen plane and the triangle indicates that the bond is coming out of the screen plane.

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Molecular Shapes: Valence Shell Electron Pair Repulsion

A molecule can be described in terms of the distribution of the bonding atoms about the central atom:

Molecular Geometry (MG)

A molecule can be described in terms of the distribution of the bonding pair electrons (bp) and lone pair electrons (lp) about the central atom:

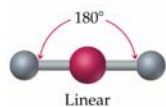
Electronic Geometry (EG)

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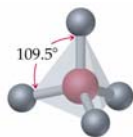
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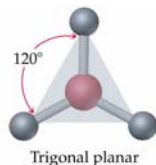
There are three fundamental shapes that describe the *geometries* for molecular shape:



2 pairs of electrons



4 pairs of electrons



(triangular)

3 pairs of electrons

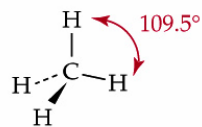
balloons time!

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4 bonding pairs of electrons about the central atom, no lone pairs:

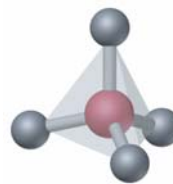


Methane: CH₄

4 groups of electrons (all bonding)

Electronic Geometry: *Tetrahedral*

Molecular Geometry: *Tetrahedral*



Tetrahedral

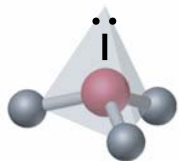
When there are no lone pairs of electrons in a molecule, the *molecular* and *electronic* geometries are the same!

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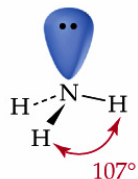
4 total pairs of electrons about the central atom, three bonding, one lone pair:



Trigonal pyramidal

Ammonia: NH_3

Molecular Geometry (MG):
Trigonal pyramidal
Electronic Geometry (EG)
Tetrahedral



4 groups of electrons (3 bp, 1 lp)

Electronic Geometry: **Tetrahedral**

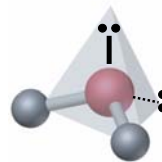
Molecular Geometry: **Trigonal Pyramidal**

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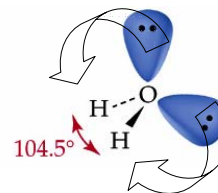
4 total pairs of electrons about the central atom, two bonding, two lone pair:



Bent

Water: H_2O

Molecular Geometry (MG):
Bent
Electronic Geometry (EG)
Tetrahedral



4 groups of electrons (2 bp, 2 lp)

Electronic Geometry: **Tetrahedral**

Molecular Geometry: **Bent**

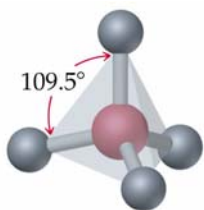
The lone pairs force the bonding atoms to bend.

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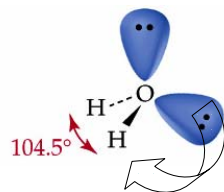
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Water: H_2O



Tetrahedral



The lone pairs force the bonding atoms to bend.

Notice that the molecular bond angles decrease as more lone pairs are added to the central atom.

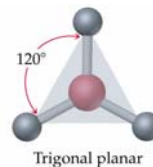
This is due to the greater lp-lp repulsion which forces the bonding atoms to move closer to one another.

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Molecules with 3 regions of electron density:



Trigonal planar

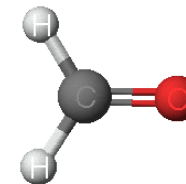
The bonds (and lone pairs) spread out in a plane to form 120° angles.

Example: CH_2O (formaldehyde)

3 groups of electrons (3 bonds, 0 lp)

Electronic Geometry: **Trigonal Planar**

Molecular Geometry: **Trigonal Planar**



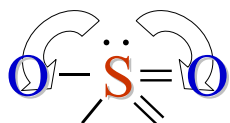
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The lone pair of electrons forces the molecule into a bent molecular geometry.



3 groups of electrons (2 bonds, 1 lp)

Electronic Geometry: *Trigonal Planar*

Molecular Geometry: *bent*

POLARITY OF COVALENT MOLECULES

The sharing of electrons in covalent bonds is not always equal between the bonding atoms.

Electrons in a covalent bond are attracted toward atoms of highest *electronegativity*.

Electronegativities for the common representative elements

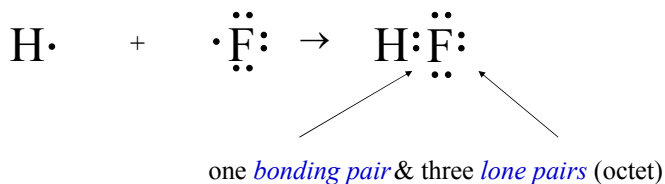
		Increasing electronegativity →						
		H						
		2.1						
Li	Be	B	C	N	O	F		
1.0	1.5	2.0	2.5	3.0	3.5	4.0		
Na	Mg	Al	Si	P	S	Cl		
0.9	1.2	1.5	1.8	2.1	2.5	3.0		
K	Ca	Ga	Ge	As	Se	Br		
0.8	1.0	1.6	1.8	2.0	2.4	2.8		
Rb	Sr	In	Sn	Sb	Te	I		
0.8	1.0	1.7	1.8	1.9	2.1	2.5		
Cs	Ba							
0.7	0.9							

↓ Decreasing electronegativity

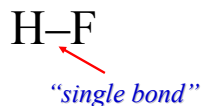
As a result the bond is said to be polarized.

When other covalent species form, there are additional electron pairs that do not participate in bonding.

These are called "*lone pairs*" (*lp*)



hydrogen fluoride: HF



Fluorine has a larger electroegativity value than hydrogen.

This means that the electrons in the bond are skewed toward the F-atom.

TABLE 4.4 Electronegativities for the common representative elements

		Increasing electronegativity →						
		H						
		2.1						
Li	Be	B	C	N	O	F		
1.0	1.5	2.0	2.5	3.0	3.5	4.0		
Na	Mg	Al	Si	P	S	Cl		
0.9	1.2	1.5	1.8	2.1	2.5	3.0		
K	Ca	Ga	Ge	As	Se	Br		
0.8	1.0	1.6	1.8	2.0	2.4	2.8		
Rb	Sr	In	Sn	Sb	Te	I		
0.8	1.0	1.7	1.8	1.9	2.1	2.5		
Cs	Ba							
0.7	0.9							

↓ Decreasing electronegativity

The electrons shift toward the F-atom



This polarizes the molecule

The greater the difference in electronegativity (ΔEN) the more polar the covalent bond.

H vs. F

$$4.0 - 2.1 = 1.9$$

C vs. F

$$4.0 - 2.5 = 1.5$$

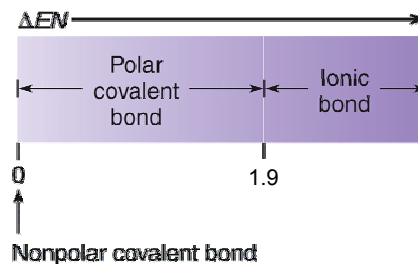
O vs. F

$$4.0 - 3.5 = 0.5$$

Li	Be	B	C	N	O	F
1.0	1.5	2.0	2.5	3.0	3.5	4.0
Na	Mg	Al	Si	P	S	Cl
0.9	1.2	1.5	1.8	2.1	2.5	3.0
K	Ca	Ga	Ge	As	Se	Br
0.8	1.0	1.6	1.8	2.0	2.4	2.8
Rb	Sr	In	Sn	Sb	Te	I
0.8	1.0	1.7	1.8	1.9	2.1	2.5
Cs	Ba					
0.7	0.9					

Decreasing electronegativity

So in terms of polarity,



*completely
molecular in
character*



*somewhere in
between
(polar covalent)*



*completely ionic
in character*