2.1 ATOMIC STRUCTURE

2.1 Assignment

1. Chemical bonds are formed when atoms share, donate or accept electrons. In your own words, explain how Dalton's, Thomson's and Rutherford's models do not allow for chemical bonding.

Dalton's model- did not know about subatomic particles yet; therefore, there were no electrons to bond

Thomson's "Plum Pudding" model- electrons and protons are scattered throughout the atom. These particles would be attracted to one another and it would be hard to remove an electron

Rutherford's "Nuclear model"- getting there, but only one sphere around the nucleus would become an issue as the number of electrons increase

Rutherford's "Solar System" model- electrons would be attracted to the positive nucleus and would cause the atom to collapse.

2. The Bohr model is useful for representing electron shells, however, this model has been replaced by the Quantum Mechanical Model. Explain how this is more accurate representation of the atom.

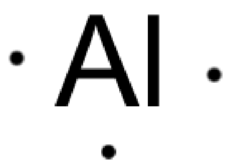
deBroglie and Schrodinger contributed to the quantum mechanical model. With these scientists came the fact that electrons can act like a wave and a particle (wave-particle duality) and the Schrodinger equation. This helps explain electron movement within an atom. Schrodinger also used a mathematical equation to predict the location of an electron (resulting in the "cloud" or 3D nature of the shell). The Bohr model assumed that electrons existed in specific energy levels and moved in a 2D motion.

3. Use the characteristics of the atoms described above, and the examples given below to complete the following chart.

Atom	Closet Noble Gas	Most Common Ion
a. Sodium	Neon	Na^{+}
b. Chlorine	Argon	Cl^{-}
c. Silicon	Neon or Argon	Si^{4+} or Si^{4-}
d. Aluminum	Neon	Al^{3+}
e. Oxygen	Neon	O^{2-}

2.1 ATOMIC STRUCTURE

4. Draw the Lewis Dot Diagrams for the **atoms** below:
    - Aluminum



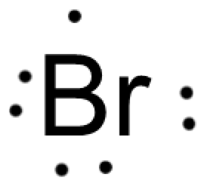
    - Calcium

    - Sulfur

    - Silicon

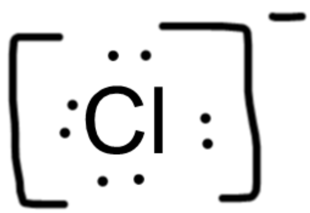
    - Neon

- Bromine

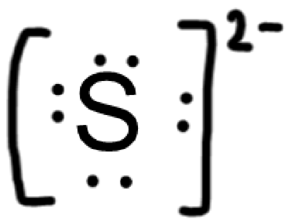


5. Draw the Lewis Dot Diagrams for the **ions** below:
   - Al^{3+}

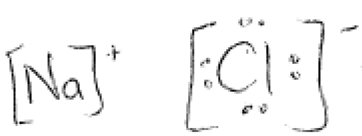
   - Cl^{-}



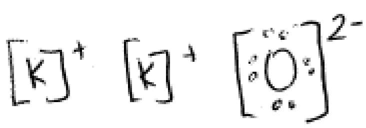
   - S^{2-}



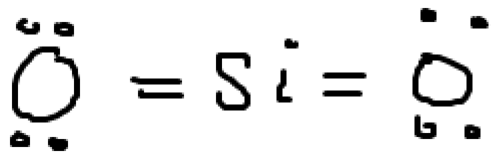
6. CHALLENGE! Draw the Lewis Structure for the following **compounds**. Hint: to begin, determine if the compound is ionic or covalent.
   - Sodium Chloride



   - Potassium Oxide

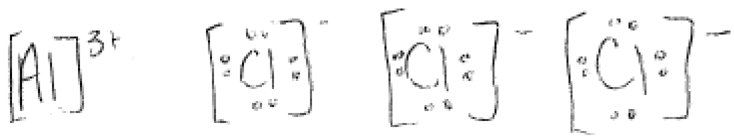


- Silicon dioxide

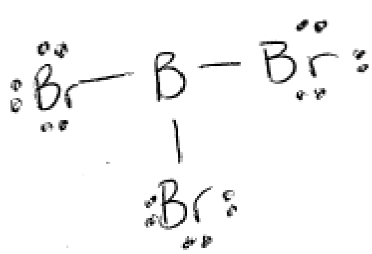


- Oxygen gas

- Aluminum chloride



- Boron Tribromide



2.1 Atomic Structure

Review of Terminology

The following is a list of words and terms that you should be familiar with. Use your textbook or other resources to help define these terms using words and a diagram or an example:

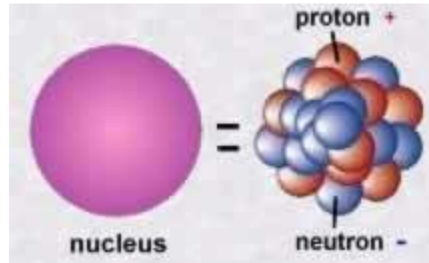
Term	**Definition**	**Diagram/Example**
1. atom		
2. nucleus		
3. electron		
4. proton		
5. ion		
6. energy level (electron shell)		
7. valence electron		

2.1 Atomic Structure

<u>Components of an Atom</u>

The modern atom as viewed by scientists today consists of three main particles located in two regions.

1. The nucleus or central core of the atom
   - is composed of **positively charged protons** and **neutrons with a neutral charge.**
   - It is believed that the neutrons are needed to hold the positively charged protons together in the nucleus.
   - The force that holds these particles together is termed the nuclear binding force and it is believed to be one of the strongest forces that exists in nature.
   - The nucleus takes up a very small portion of the atom.



2. Electron cloud is the second region and surrounds the nucleus.
   - The cloud holds the **third particle, which is a negatively charged electron.**
   - Electrons circle the nucleus in the electron cloud; we never know both the location and speed of an electron (*Heisenberg's Uncertainty Principle*)
   - However, we do know the electrons are arranged in energy levels about the nucleus.
   - The electrons in their lowest energy state (termed ground state) occupy these energy levels from lowest (closest to nucleus) to highest energy.
   - Only certain numbers of electrons can be placed in each energy level; thus, we can take an estimated guess as to the location of a specific electron in general.

Ions: The number of electrons in a neutral atom (no charge) is equal to the number of protons (atomic #). Atoms may either gain or lose electrons during chemical interactions with other atoms. If they gain electrons they become negatively charged, if they lose electrons they become positively charged. We term these charged atoms ions.

For Example: If Magnesium loses two electrons it would have 12 + charged protons and only 10 - charged electrons and would become a +2 ion. If Chlorine gains one electron it would have 35 protons (+) and 36 electrons (-) and become a - 1 ion. The charge on the ion indicates the number of electrons gained or lost.

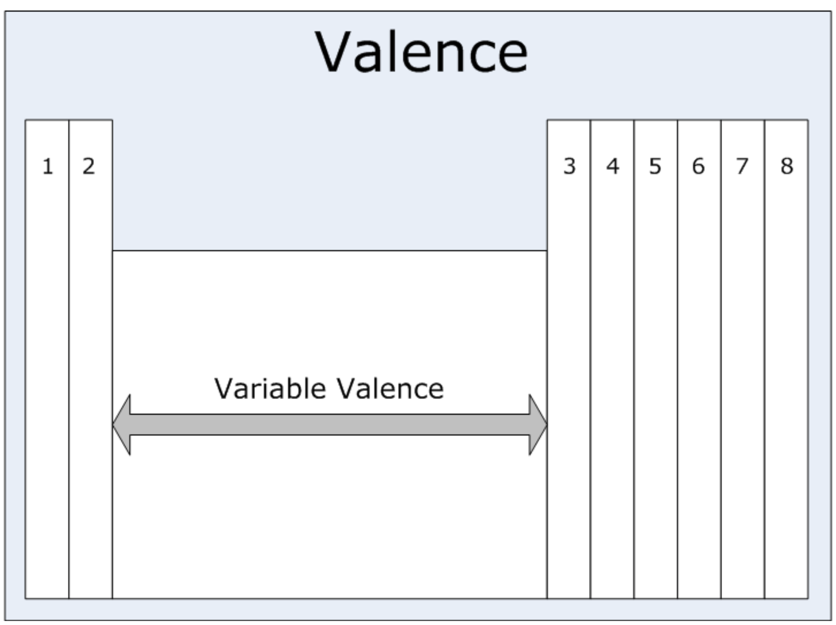
Electron Dot Diagrams:

- The *octet rule* states that atoms are most stable when they have a full shell of electrons in the outside electron ring (or energy level).
  - The first shell has only two electrons in a single subshell. Helium has a full shell, so it is stable, an inert element. Hydrogen, though, has only one electron. It can lose an electron to become H+, a hydrogen ion or it can gain an electron to become H-, a hydride ion.
  - All the other shells have 2 subshells, giving them at least eight electrons on the outside. These subshells often are the only valence electrons, thus the octet rule is named for the eight electrons found here.
  - The Transition Elements, Lanthanides, and Actinides are all metals. Many of them have varying valences because they can trade around electrons from the outer shell to the inner subshells (these elements can have up to 4 subshells in energy levels 4-6) that are not filled. For this reason they sometimes appear to violate the octet rule.

- **Valence electrons are the electrons in the outermost shell of the atom.** These are the electrons most likely to interact when chemical reactions occur and are therefore of great interest to chemists. (refer to periodic table)

<u>Electron Arrangement and the Periodic Table</u>

The columns in the periodic table represent the number of valence electrons an atom has to work with. The table below illustrates these numbers. We can use these number to draw Lewis Dot Diagrams predict an atoms chemical behavior.



For example, Magnesium **For example, Polonium**

2.1 Assignment

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2. The Bohr model is useful for representing electron shells, however, this model has been replaced by the Quantum Mechanical Model. Explain how this is more accurate representation of the atom.

3. Use the characteristics of the atoms described above, and the examples given below to complete the following chart.

Atom	Closet Noble Gas	Most Common Ion
a. Sodium	Neon	Na^+
b. Chlorine		
c. Silicon		
d. Aluminum		
e. Oxygen		

4. Draw the Lewis Dot Diagrams for the **atoms** below:
   - Aluminum
   - Calcium
   - Sulfur
   - Silicon
   - Neon
   - Bromine

5. Draw the Lewis Dot Diagrams for the **ions** below:
   - Al^{3+}
   - Cl^{-}
   - S^{2-}

6. CHALLENGE! Draw the Lewis Structure for the following **compounds**. Hint: to begin, determine if the compound is ionic or covalent.
   - Sodium Chloride
   - Potassium Oxide
   - Silicon dioxide
   - Oxygen gas
   - Aluminum chloride
   - Boron Tribromide

2.1-2.3 Hand In Assignment /38

1. Describe **the difference** between at atom and an ion in regards to their substaomic particles. (1)

2. Draw the Lewis Dot Diagram for the following atoms and ions:
   a. Aluminum (atom and ion) (2)

   b. Chlorine (atom and ion) (2)

3. In terms of potential energy, state why atoms tend to bond in nature (1).

4. Which member of each of the following pairs would you expect to have the higher melting point? **Explain your reasoning.** (1 each)
   a. CaO or RbI

   b. LiF or NaCl

   c. CH4 or CH3Cl

5. Using H2O as your example, illustrate the difference between intermolecular and intramolecular forces (be specific as to what types of forces/bonds are being observed in water) (4).

6. <u>Explain</u>, two differences **between the properties** of ionic and covalent (molecular) compounds. (4)

7. How is it possible for a molecule to be nonpolar if it contains polar bonds? Use an example to support your explanation (2).

8. In column A, record the electronegativity difference in each molecule. In column B, intramolecular force contained in each molecule. In column C, tell me the intermolecular force acting between molecules. (3)

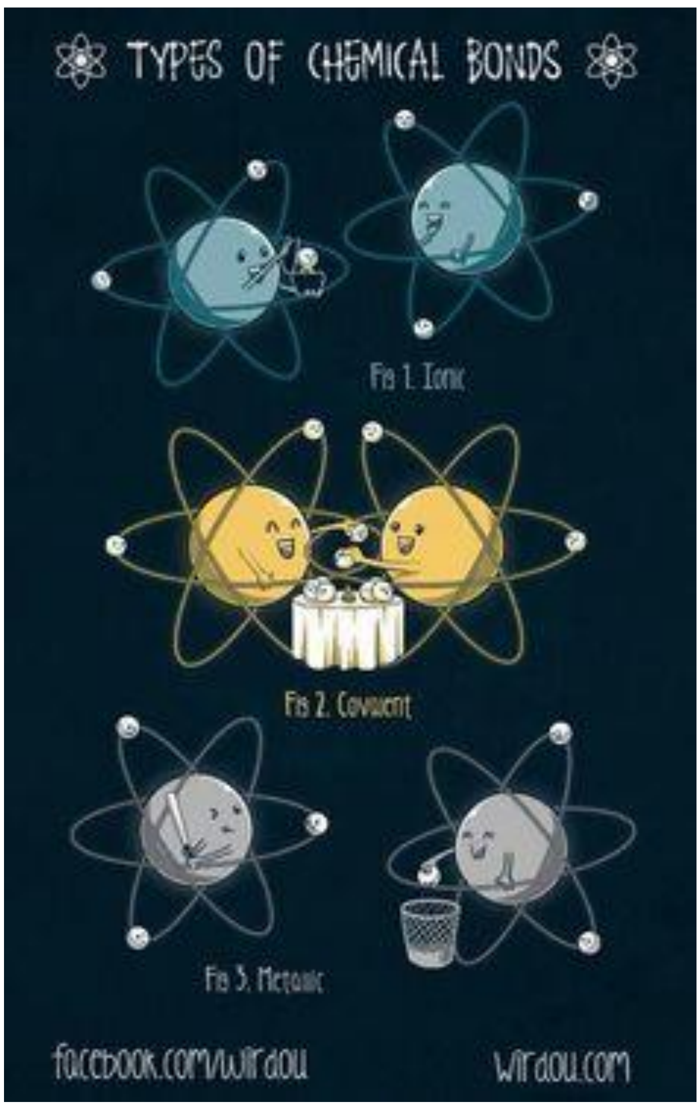
Molecule	Column A	Column B	Column C
1. NaF			
2. NI3			

9. Complete the following table (4 each)

Molecule DRAW LEWIS STRUCTURE HERE	**Molecular Geometry (VSEPR shape)**	**VSEPR Drawing**	**Polar/Non polar/ charged?**
BCl_3			
ClF_3			
XeF_2			
$[NH_4]^+$			

Chemistry 30
Chemical Bonding

For additional help, check out pages 328-438 in Heath Chemistry



Chemical Bonding ANSWER KEY

Ionic Bonds

1. Define the following terms:
   a) ionic bond – a type of bond between a metal and a non-metal that involves the transfer of electrons to create ions
   b) crystal – a structure with regular repeating patterns

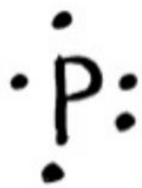
Reviewing Lewis Dot Diagrams for Ions

Write the Lewis Dot Diagrams for the following:

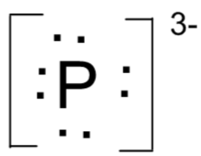
beryllium atom:

beryllium ion:

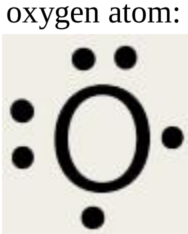
phosphorus atom:



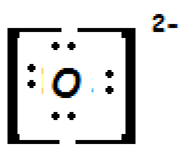
phosphide ion:



oxygen atom:

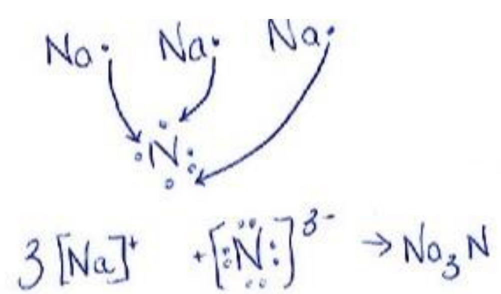


oxide ion:

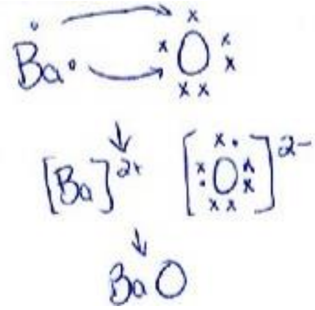


Drawing Ionic Bonds

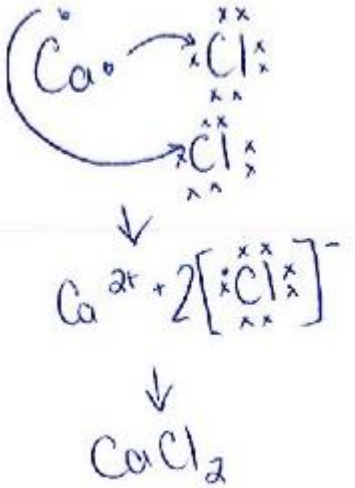
1. sodium nitride



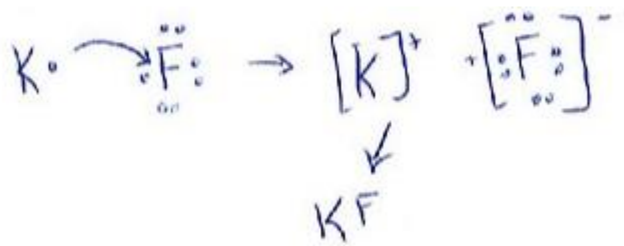
2. barium oxide



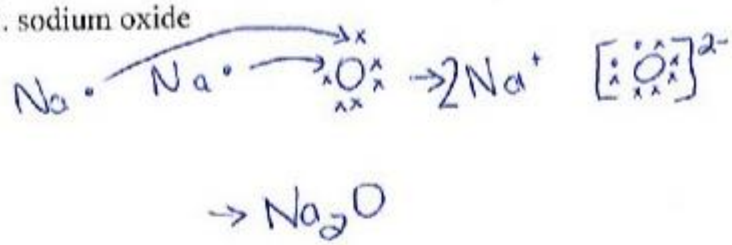
3. calcium chloride



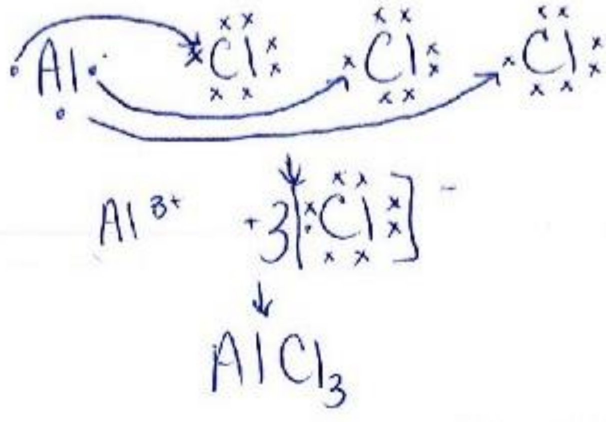
4. potassium fluoride



5. sodium oxide



6. aluminum chloride



Introduction to Covalent Bonds

1. Define the following terms:
   a) covalent bond – a bond formed between two non-metals in which electrons are shared

   b) molecule – a particle that contains two or more atoms that is electrically neutral

   c) intramolecular force– forces inside the molecule that hold the molecule together (ie. Covalent bond)

   d) intermolecular force– forces between molecules that hold one molecule to another

2. Define the following terms:

   a) single covalent – 2 electrons are shared in a covalent bond

   b) double covalent – 4 electrons are shared in a covalent bond

   c) triple covalent – 6 electrons are shared in a covalent bond

3. What type of bonding exists in network solids?

   *Covalent bonding exists in network solids within molecules and between molecules.

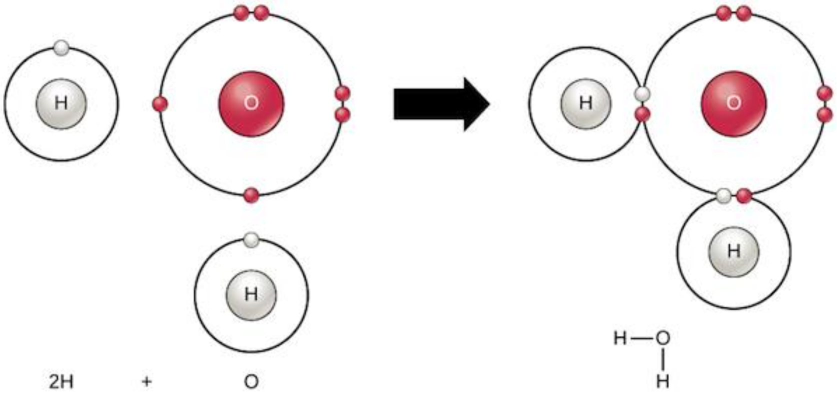
4. List two ways in which a network covalent solid is similar to an ionic compound.

   1. There are forces between molecules holding them together
   2. They form a crystalline pattern

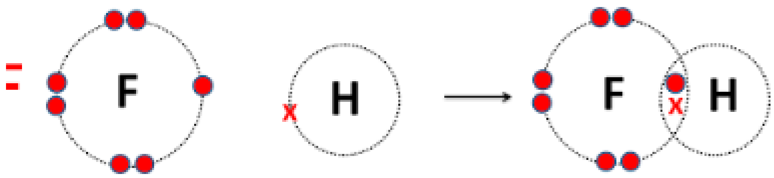
Drawing Covalent Bonds

1. Chlorine and chlorine

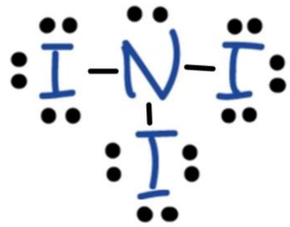
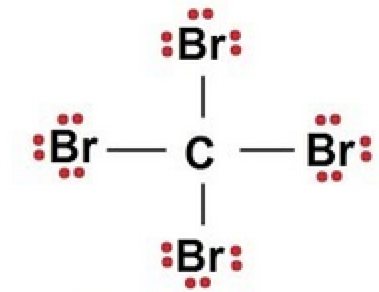
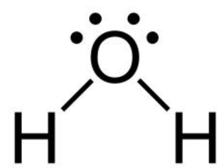
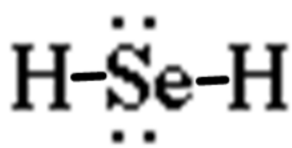
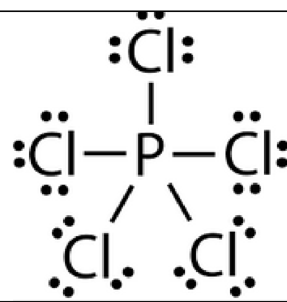
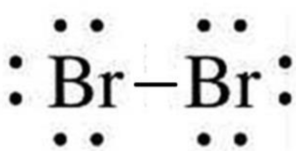
2. Hydrogen and oxygen forming water (H_2O)



3. Hydrogen and fluorine (HF)

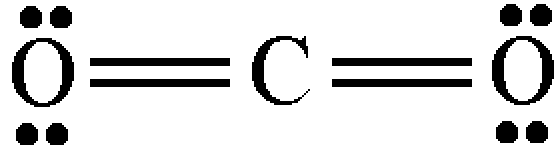
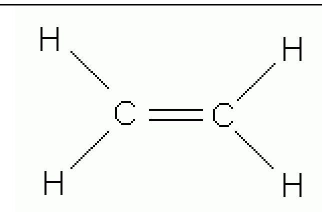


Drawing Single Covalent Bonds

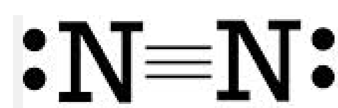
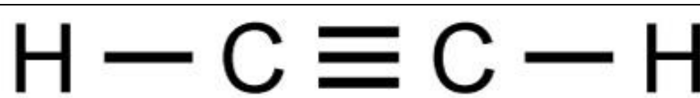
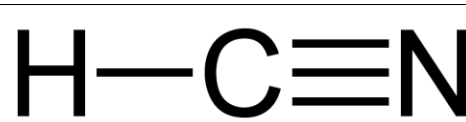
Work	Final Answer
Ex: nitrogen triiodide (NI_3) N(5) + I (7x3) = 26ve	
1. carbon tetrabromide (CBr_4)	
2. dihydrogen monoxide (H_2O)	
3. dihydrogen monoselenide	
4. phosphorus pentachloride	
5. Bromine gas	

Double AND Triple Covalent Bonds

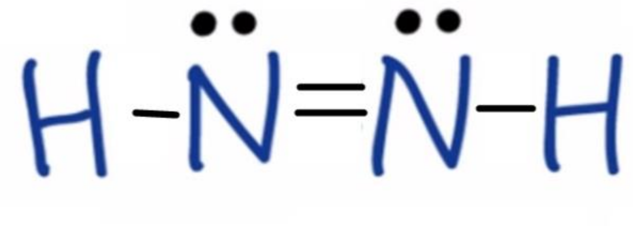
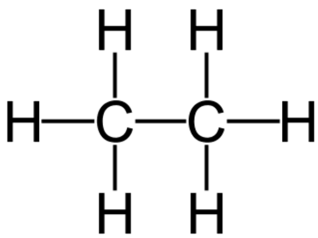
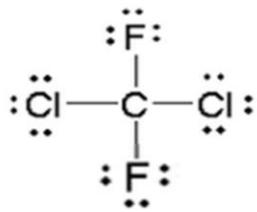
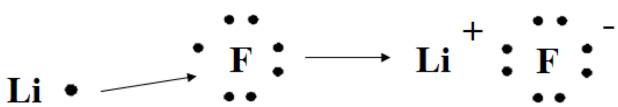
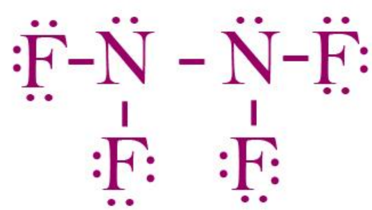
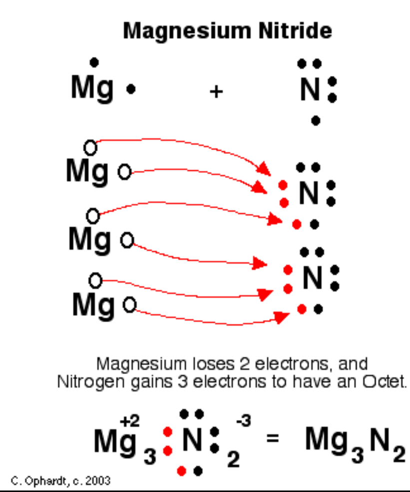
Double bonds can form when a shared single bond alone doesn't satisfy either atoms valence. Double bonds are TWO SHARED PAIRS of electrons for a total of 4 electrons (2 electrons from one atom and 2 from the other). Double bonds are much stronger and bond the atoms closer than a single bond.

Work	Final Answer
Ex: carbon dioxide C(4) + O(6x2) = 16ve	
1. Oxygen gas	
2. Ethene (C_2H_4) ** C's are always central and they will link together.	

Triple bonds can form when 3 pairs of electrons are shared for a total of 6 shared electrons. Typically, one atom donates 3 electrons and the other atom donates the other 3. Triple bonds are even stronger than double bonds and the atoms are held even closer together.

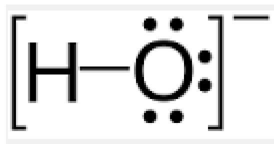
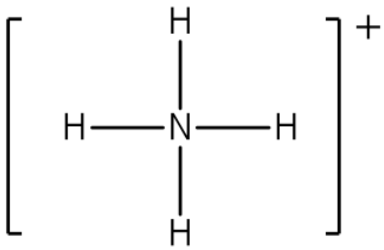
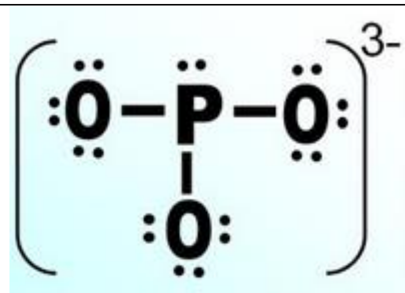
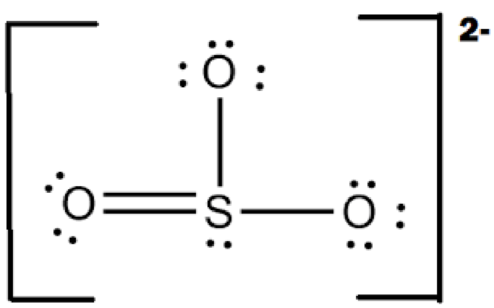
Work	Final Answer
Ex: Nitrogen gas N(5x2) = 10ve	
1. Ethyne (C_2H_2) ** C's are always central and they will link together.	
2. hydrogen cyanide (HCN)	

A mixture of all types of bonds: Draw the bonding diagrams (using arrows for ionic and Lewis Structures for covalent).

Work	Final Answer
1. N_2H_2	
2. C_2H_6	
3. CF_2Cl_2	
4. LiF	
5. N_2F_4	
6. Mg_3N_2	

Polyatomic Ions

Now you are going to draw electron dot diagrams for the following polyatomic ions. Remember that even though they are ions, the atoms are held together inside the ion with covalent bonds. Negative ions have gained electrons, you must include these in the structure. Positive ions have lost electrons, you must delete these from the structure.

Work	**Final Answer**
Ex. hydroxide ion $[OH]^{-1}$ H(1) + O(6) +1 = 8ve	
1. ammonium ion $[NH_4]^{+1}$	
2. phosphite ion $[PO_3]^{-3}$	
3. sulfite ion	

Polarity and Electronegativity

1. Define the following terms:

   a. polar covalent-covalent bond with unequal sharing of electrons

   b. nonpolar covalent- covalent bond with equal sharing of electrons

1. Sodium chloride (NaCl) is an example of an ionic bond. What is the difference in electronegativity between sodium and chlorine? A: 2.1

2. Nitrogen dioxide (NO_2) is an example of a covalent bond. What is the difference in electronegativity between nitrogen and oxygen? A: 0.5

3. Use the table and chart from this worksheet to label the following bond types as nonpolar, polar or ionic:

a. NH_3

0.9 difference; therefore, polar covalent

b. MgO

2.3 difference; therefore, ionic

c. Cl_2

0 difference; therefore, nonpolar covalent

d. HCl

0.9 difference; therefore, polar covalent

e. H_2O

1.4 difference; therefore, polar covalent

f. NaCl

2.1 difference; therefore, ionic

g. CH_4

0.4 difference; therefore, non-polar covalent

h. NO_2

0.5 difference; therefore, polar covalent

Metallic Bonds

1. What is a metallic bond? Explain how the ions and electrons are arranged.
A metallic bond is formed between multiple metal atoms with electrons being delocalized between all of the atoms involved.

2. What is an alloy?
An alloy is a mixture of metals that contains metallic bonds.

3. Identify the following compounds as metallic, ionic or covalent:

a. RbCl-ionic

b. Cl_2-covalent

c. Au -metallic

d. $[BrO_3]^{-1}$ - covalent

e. Mg_3N_2 -ionic

f. Pt -metallic

g. Al - metallic

h. Ag -metallic

Intermolecular (van der Waals) Forces

1. List the van der Waals forces in order of increasing strength.

H—bonding > Dipole-Dipole >London Dispersion Forces

2. Explain instantaneous dipoles and how this results in a weak intermolecular force.
Electrons are shared unevenly in a nonpolar bond (momentarily), which causes an unequal distribution in a neighboring molecule…causing a brief attraction between the normally non-polar bonds.

Use your electronegativity table and the chart above to answer the following questions:

1. Determine the INTRAmolecular force for the following compounds: (nonpolar covalent, polar covalent, ionic)

CH_4 = nonpolar covalent CF_4= polar covalent HI = nonpolar covalent

CO_2 = polar covalent NH_3= polar covalent NaCl = ionic

2. Determine the INTERmolecular force for the compounds above: (London forces, dipole-dipole, H bonding, ionic)

CH_4 = London forces CF_4= dipole-dipole HI = London forces

CO_2 = dipole-dipole NH_3= H bonding NaCl = ionic

2.2 Assignment

Bonding Vocabulary Review Sheet
Give the type of bond or force described by the following:

Your choices can be (and you will use some them more than once):
Covalent **Metallic Bond** **Network Solid**
Ionic bond **Van der Waals**

Ionic bond	1.	This bonding is found between cations and anions.
Covalent Bond	2.	This is found between atoms of nonmetals.
Metallic Bond	3.	This is found between atoms of metals.
Network Solid	4.	This is the force that holds quartz together.
Van der Waals	5	This is a term to describe all intermolecular forces.
Metallic Bond	6.	This is the force that produces electrical conductivity in the solid state.
Ionic bond	7.	This is the force that produces an electrical insulator in the solid state but an electrical conductor in the liquid state.
Ionic bond	8.	This is the force that holds crystals of table salt together.
Network Solid	9.	This is the force that holds a diamond together.

Your choices can be (and you will use some them more than once):
Polar Covalent **Hydrogen Bond** **London Force**
Nonpolar Covalent **Dipole-Dipole Force** **Ionic Bond**

Dipole-Dipole Force	10.	This is the term to describe the attraction between one polar molecule and another polar molecule.
London Force	11.	This is the term to describe the attraction between one nonpolar molecule and another nonpolar molecule.
Nonpolar Covalent	12.	This is the force inside a molecule of bromine (holds **the** molecule together).
London Force	13.	This is the force between two molecules of bromine (holds molecul**es** together).
Nonpolar Covalent	14.	This is the force inside a molecule of methane CH_4.
London Force	15.	This is the force between two molecules of methane CH_4.
Ionic	16.	This is the force that holds cesium fluoride together.
Polar Covalent	17.	This is the force that holds the carbon to the oxygen in carbon dioxide.
Polar Covalent	18.	This is the force inside a water molecule (H_2O)
Hydrogen Bond	19.	This is the force between water molecules.
Nonpolar Covalent	20.	This is the force inside a molecule of nitrogen (N_2).

London Force 21. This is the force between two molecules of nitrogen.

22. Explaining the Properties of Ionic Compounds
Using what you know about ionic bonds and crystal structure, complete the following sentence stems.

Ex. Ionic compounds have relatively high melting and boiling points because…their ions are held together by strong forces (ionic bonds).

1. Ionic compounds are hard because …they have strong intramolecular bonds.
2. A piece of sodium chloride is easily cracked or fractured because…the crystal lattice structure becomes offset when the crystal is hit; this can cause positive ions to be next to each other which would create a repulsive force between like charges-breaking the lattice.
3. Ionic compounds are electrolytes because…the compound dissociates in water and ions (electrons) are able to move freely and can therefore carry an electric charge through the water.

23. Explaining the Properties of Covalent Compounds
Using what you know about covalent bonds, complete the following sentence stems.

Ex. Covalent compounds are usually liquids or gases at room temperature because…there is little attraction between molecules (London dispersion forces)

1. Covalent compounds are share electrons because …they are made up of non-metals that like to keep their electrons to fill their outer shell (octet rule).
2. A piece of paraffin wax is easily malleable because…there are weak intermolecular forces between the molecules (London Dispersion).
3. Covalent compounds are weak electrolytes because…they don’t dissociate in water and the electrons cannot move freely to carry the electric charge.

24. Explaining the Properties of Metallic
Using what you know about metallic bonds, complete the following sentence stems.

Ex. Metallic compounds are malleable and ductile because… metal crystal structures are flexible (layers within the crystal lattice can slide across one another).

1. Metallic compounds conduct electricity because …delocalized electrons are mobile within the solid.
2. Metallic compounds are insoluble because…this would mean electrons have to be localized to one atom in order to separate the atoms; this is very hard to do and therefore, metals are insoluble.
3. Metallic compounds are usually solid at room temperature because …metallic bonds are very strong.

25. Bonding Multiple Choice Review Sheet

For questions 1-30 the choices are:

(1) ionic (2) polar covalent (3) nonpolar covalent (4) metallic (5) van der Waals forces
*** If you use this, be specific on WHICH van der Waals force.

1. The bonding found in calcium chloride is …1

2. The bonding found in silver is …4

3. The bonding found inside a molecule of carbon tetrachloride is …2

4. The bonding that holds water molecules together to make ice is …5 (H-bonding)

5. The bonding found in a high melting point crystalline solid that conducts electricity when liquid…1

6. The bonding found between atoms in carbon disulfide is …3

7. The bonding found in a molecule of ammonia (NH_3) is …2

8. The intramolecular force in iodine (I_2) is …3

9. The intermolecular force in iodine is …5 (London Dispersion)

10. The bonding found is sodium fluoride is …1

13. The bonding that produces electrical conductivity in the solid state is …4

14. The bonding found in a network solid is either … or … 2 or 3

15. The bonding found in any alloy is …4

16. The bonding that results from the complete transfer of electrons is …1

17. The bonding that is an equal sharing of valence electrons is …3

18. The bonding between elements with an electronegativity difference of 1.75 is …1

19. The bonding within a sulfate ion is …2

20. The bonding between sodium and sulfate in sodium sulfate is …1

21. The bonding within hydrocarbon molecules (made of hydrogen and carbon) is … 3

22. The bonding between hydrocarbon molecules is …5 (London Dispersion)

23. The bonding that depends upon a loose cloud of valence electrons or an “electron glue” is …4

24. The bonding that creates dipoles is …2

For questions 25-35 the choices are:
(1) single covalent (2) double covalent (3) triple covalent (4) hydrogen bonding (5) London forces

25. The bonding that results from the formation of "instantaneous dipoles" is …5

26. The intramolecular forces in liquid nitrogen (N_2) are …3

27. The intermolecular forces in liquid nitrogen are …5

28. Acetylene (C_2H_2) has the carbons bonded to each other and one hydrogen bonded to each carbon. The bonding between the carbon atoms is …3

29. The attraction of a hydrogen atom in one molecule for a more electronegative element in another molecule is what we call …4

30. The strongest of the above choices is …3

31. The weakest of the above choices is … 5

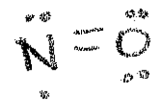
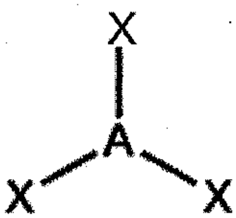
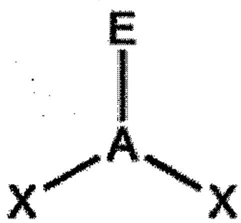
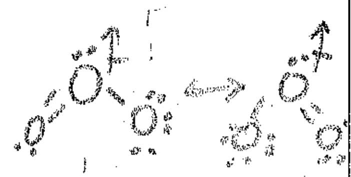
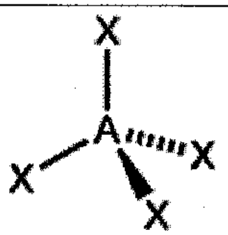
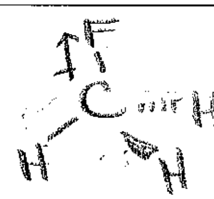
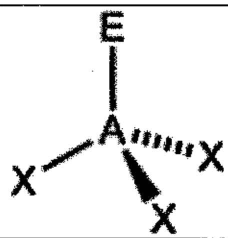
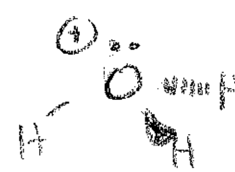
32. The bonding that is broken when you turn water into steam is … 4

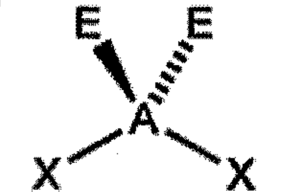
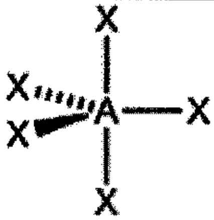
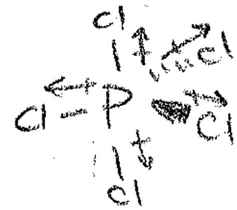
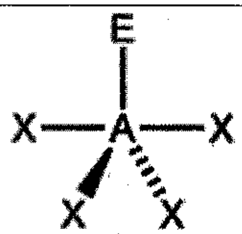
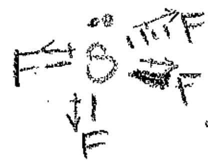
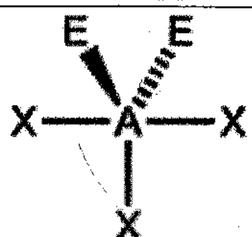
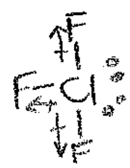
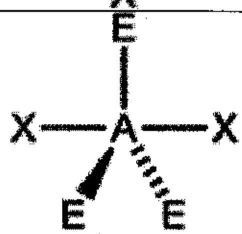
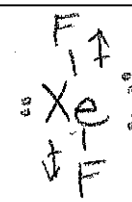
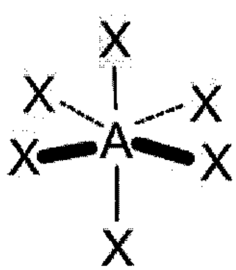
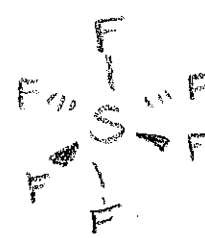
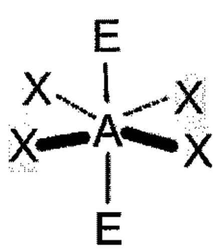
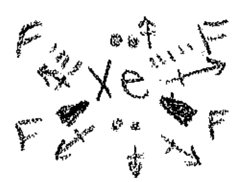
33. The bonding that is broken when you do electrolysis (splitting) of water molecules to form hydrogen and oxygen is …1

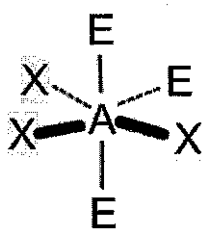
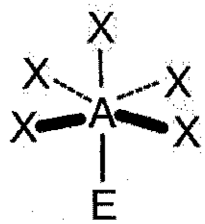
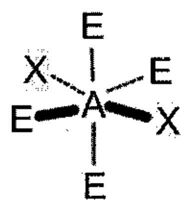
34. The intramolecular force in hydrogen chloride is …1

35. The intramolecular force in carbon monoxide is …3

Note, this table utilized the AXE method. "A" is the central atom. "X" are the bonded atoms (peripheral atoms). "E" if the unbound/lone pairs of electrons.

Shape	# Bonding Pair(s)	#Lone electron pairs	Molecular Geometry	Example **Specify whether your example is polar of nonpolar
A—X	1	0	linear	 NP
X—A—X	2	0	linear	$H-C\equiv N:$ P
	3	0	trigonal planar	 NP
	2	1	bent	 P
	4	0	tetrahedral	 P
	3	1	Trigonal pyramidal	 H_3O^+ Charged

	2	2	Bent	 P.
	5	0	trigonal bipyramidal	 NP
	4	1	seesaw	 P.
	3	2	T-shaped	 P
	2	3	linear	 NP
	6	0	octahedral	 NP
	4	2	square planar	 NP

	3	3	T-shaped	
	5	1	square pyramidal	
	2	4	Linear	

VSEPR THEORY

STUDENT LEARNING OUTCOMES:

- Learn how to draw Lewis structures for atoms which violate the octet rule.
- Learn how to use Lewis structures and VSEPR and to predict the shapes of molecules.
- Learn how to use the shape of a molecule to predict whether or not it is polar.

EXPERIMENTAL GOALS:

The purpose of this lab activity is to predict the VSEPR shape of those molecules, and whether or not the molecules are polar.

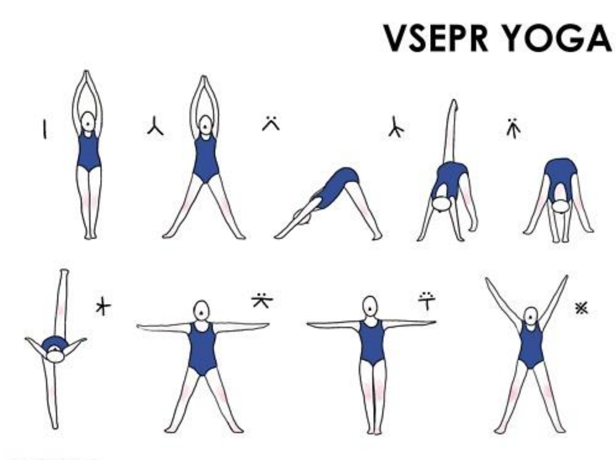
MATERIALS:

Each group of students will need a molecular modeling kit.

INTRODUCTION:

What information do you already have that can help you modify two dimensional Lewis structures into more accurate three dimensional models? You know that all electrons have the same charge and that like charges repel. It is reasonable to assume that the electron pairs in bonds will be oriented in a molecule as far from each other as possible. The valence electrons should be expected to occupy regions of space so that the shared pairs are evenly distributed around the central atom.

There are several theories in chemistry that suggest explanations for bonding in molecules. Each theory leads chemists to predict the shapes we will learn about today. The theory we will focus on is one that describes equal distribution of electron pairs around a central atom; this theory is known as the valence shell electron pair repulsion theory (VSEPR theory). To begin, we must delve into some of the exceptions that exist to the rules we learnt about in section 2.2.

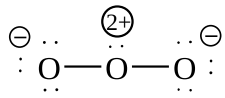


EXCEPTIONS to 2.2!
Resonance Structures — When One Lewis Structure Isn't Enough

O_3 (ozone)

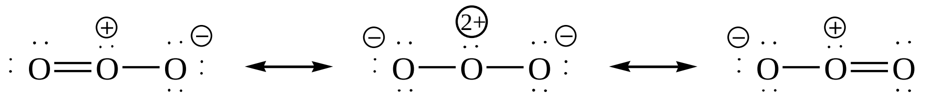
18 valence electrons (3×6)

Place one O in the center, and connect the other two O's to it. Drawing a single bond from the terminal O's to the one in the center uses four electrons; 12 of the remaining electrons go on the terminal oxygens, leaving one lone pair on the central oxygen:



1

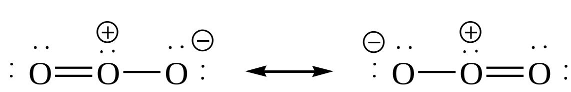
We can satisfy the octet rule on the central O by making a double bond either between the left O and the central one (**2**), or the right O and the center one (**3**):

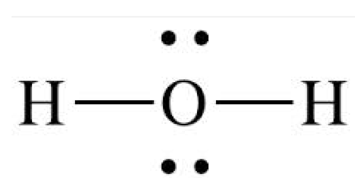


2 **1** **3**

In this example, we can draw two Lewis structures that are *energetically equivalent* to each other — that is, they have the same types of bonds, and the same types of formal charges on all of the structures, and *both structures* (**2** and **3**) are used to represent the molecule's structure. The actual molecule is an *average* of structures **2** and **3**, which are called **resonance structures**. (Structure **1** is also a resonance structure of **2** and **3**, but since it does not satisfy the octet rule, it is a higher-energy resonance structure, and does not contribute as much to our overall picture of the molecule.) Structures **2** and **3** in the example above are somewhat "fictional" structures, in that they imply that there are "real" double bonds and single bonds in the structure for ozone; in reality, however, ozone has two oxygen-oxygen bonds which are equal in length, and are halfway between the lengths of typical oxygen-oxygen single bonds and double bonds — effectively, there are two "one-and-a-half" bonds in ozone. The real molecule does *not* alternate back and forth between these two structures; it is a *hybrid* of these two forms.

The ozone molecule, then, is more correctly shown with both Lewis structures, with the two-headed resonance arrow between them:





In these resonance structures, one of the electron pairs (and hence the negative charge) is "spread out" or *delocalized* over the whole molecule. In contrast, the lone pairs on the oxygen in water (to the right) are *localized* — i.e., they're stuck in one place. Resonance delocalization stabilizes a molecule by spreading out charges. Resonance plays a large role in our understanding of structure and reactivity in organic chemistry.

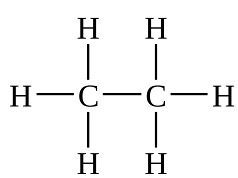
As a general rule, when it's possible to make a double bond in more than one location, and the resulting structures are energetically equivalent to each other, each separate structure must be shown, separated from each other by resonance arrows.

CO_3^{2-} (carbonate ion)

Multi-Center Molecules

Molecules with more than one central atoms are drawn similarly to the ones above. The octet rule can be used as a guideline in many cases to decide in which order to connect atoms.

1. C_2H_6



3. CH_3CH_2OH

2. C_2H_4

“Violations” of the Octet Rule

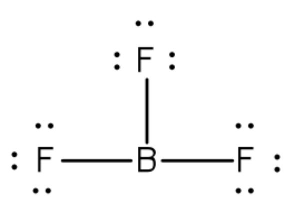
A number of species violate the octet rule by having fewer than eight electrons around the central atom or by having more than eight electrons around the central atom.

- **Electron deficient** species, such as beryllium (Be), boron (B), nitrogen (N), and aluminum (Al) can have fewer than eight electrons around the central atoms. Molecules with electron deficient central atoms tend to be fairly reactive (many electron-deficient species act as Lewis acids).
- **Free radicals** contain an odd number of valence electrons. One atom will have an odd number of electrons, and will not have a complete octet in the valence shell. As a result, these species are extremely reactive. When drawing these compounds, there are often several possible resonance structures than can be drawn.
- **Expanded valence shells** are often found in nonmetals from period 3 or higher, such as sulfur, phosphorus, and chlorine. These species can accommodate more than 8 electrons by shoving “extra” electrons into empty orbitals. Note that period 2 elements CANNOT have more than eight electrons.

Examples:

BF_3

24 valence electrons ($3 + 3\times7$)



The octet rule is not satisfied on the B, but this is the correct Lewis structure.

NO (nitrogen monoxide, or nitric oxide)

PCl_5

SF_6

XeF_4

The Shapes of Molecules (or Molecular Geometry): The VSEPR Model

Drawing a Lewis structure is the first steps towards predicting the three-dimensional shape of a molecule. The shape of molecules strongly affect their physical properties, and is very important in the way that biological molecules interact with each other.

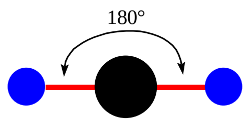
Steps to determine the shape of a molecule:

1. Draw the Lewis structure for the molecule of interest and count the number of electron groups surrounding the central atom. Each of the following constitutes an electron group:
   - a single, double or triple bond (multiple bonds count as one electron group)
   - a lone pair
   - an unpaired electron

2. Predict the arrangement of electron groups around each atom by assuming that the groups are oriented in space as far away from one another as possible.

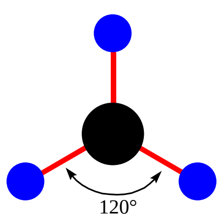
3. The shapes of larger molecules having more than one central are a composite of the shapes of the atoms within the molecule, each of which can be predicted using the VSEPR model (this is a larger scope that we will touch on in unit 3).

Two Electron Groups

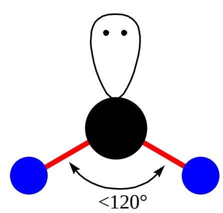


2 bonds, 0 lone pairs
linear
bond angles of 180°

Three Electron Groups



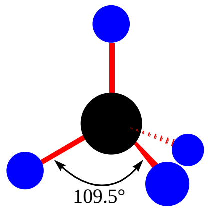
3 bonds, 0 lone pairs
trigonal planar
bond angles of 120°



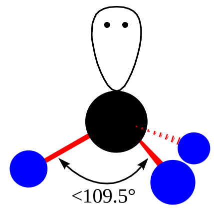
2 bonds, 1 lone pair
bent
bond angles of < 120°

Lone pairs take up more room than covalent bonds; this causes the other atoms to be squashed together slightly, decreasing the bond angles by a few degrees.

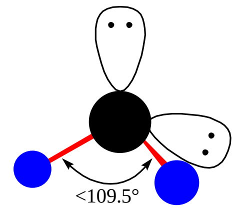
Four Electron Groups



4 bonds, 0 lone pairs
tetrahedral
bond angles of 109.5°



3 bonds, 1 lone pair
trigonal pyramidal
bond angles of <109.5°

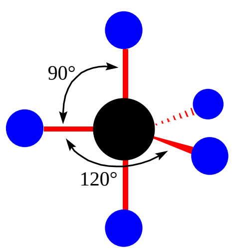


2 bonds, 2 lone pairs
bent or angular
bond angles of <109.5°

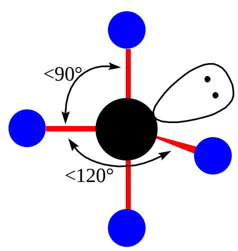
****Note****

A dashed line means that bond is going backwards into the page you are viewing. A solid line means that bond is found on the same plane as the page you are looking at. A bolded line means that bond is coming forward out of the page you are viewing.

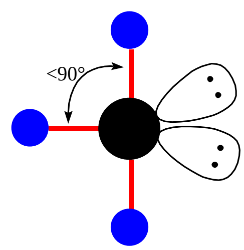
Five Electron Groups



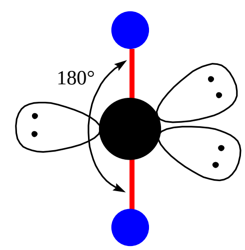
5 bonds, 0 lone pairs
trigonal bipyramidal
bond angles of 120° (equatorial), 90° (axial)



4 bonds, 1 lone pair
Seesaw or sawhorse
bond angles of <120° (equatorial), <90° (axial)

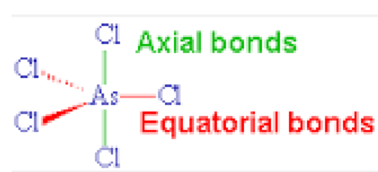


3 bonds, 2 lone pairs
T-shaped
bond angles of <90°



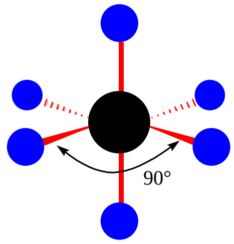
2 bonds, 3 lone pairs
linear
bond angles of 180°

The trigonal bipyramidal shape can be imagined as a group of three bonds in a trigonal planar arrangement separated by bond angles of 120° (the *equatorial* positions), with two more bonds at an angle of 90° to this plane (the *axial* positions).

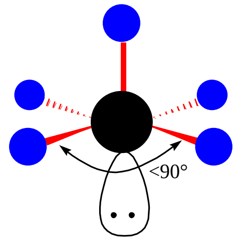


Lone pairs go in the equatorial positions, since they take up more room than covalent bonds. In the equatorial position, lone pairs are ~120° from other bonds, while in the axial positions they would be 90° away from other bonds.

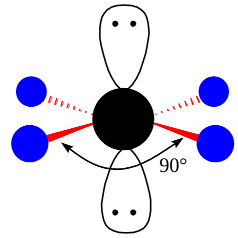
Six Electron Groups



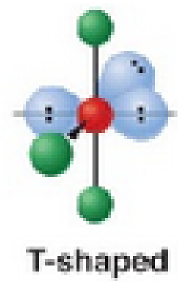
6 bonds, 0 lone pairs
octahedral
bond angles of 90°



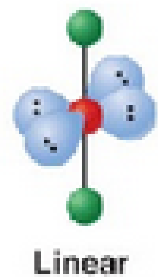
5 bonds, 1 lone pair
square pyramidal
bond angles of <90°



4 bonds, 2 lone pairs
square planar
bond angles of 90°



3 bonds, 3 lone pairs
T-shaped
bond angles of <90°



2 bonds, 4 lone pairs
Linear
bond angles of 90° and 180°

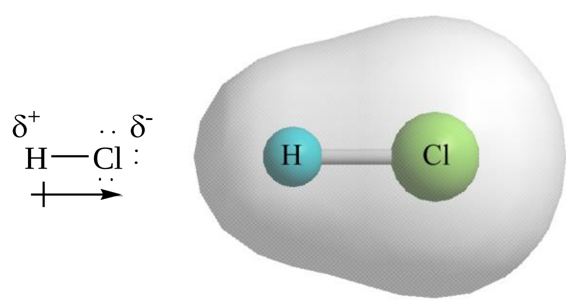
Examples

Methane (CH_4)

Carbon Dioxide (CO_2)

Polar and Nonpolar Covalent Bonds

Remember that when two bonded atoms have a difference of between 0.5 and 1.69 electronegativity units, the electrons are shared *unequally*, and the bond is a **polar covalent bond** — there is an *unsymmetrical* distribution of electrons between the bonded atoms, because one atom in the bond is "pulling" on the shared electrons harder than the other, but not hard enough to take the electrons completely away (as in an ionic bond). The more electronegative atom in the bond has a **partial negative charge** (δ^-), because the electrons are pulled slightly towards that atom, and the less electronegative atom has a **partial positive charge** (δ^+), because the electrons are partly (but not completely) pulled away from that atom. For example, in the HCl molecule, chlorine is more electronegative than hydrogen by 0.96 electronegativity units. The shared electrons are pulled slightly closer to the chlorine atom, making the chlorine end of the molecule very slightly negative (indicated in the figure below by the larger electron cloud around the Cl atom), while the hydrogen end of the molecule is very slightly positive (indicated by the smaller electron cloud around the H atom), and the resulting molecule is polar:

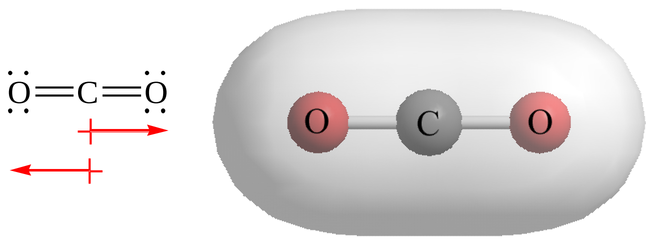


Molecular Shape and Polarity

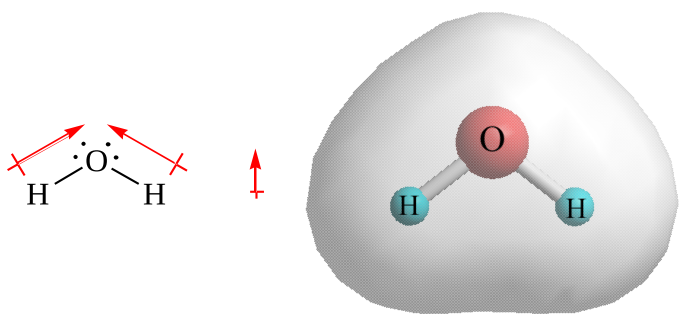
In a diatomic molecule, there is only one bond, and the polarity of that bond determines the polarity of the molecule: if the bond is polar, the molecule is polar, and if the bond is nonpolar, the molecule is nonpolar.

In molecules with more than one bond, *both shape and bond polarity determine whether or not the molecule is polar*. A molecule must contain polar bonds in order for the molecule to be polar, but if the polar bonds are aligned exactly opposite to each other, or if they are sufficiently symmetric, the bond polarities **cancel out**, making the molecule nonpolar. (Polarity is a vector quantity (think back to science 10), so both the magnitude and the *direction* must be taken into account.)

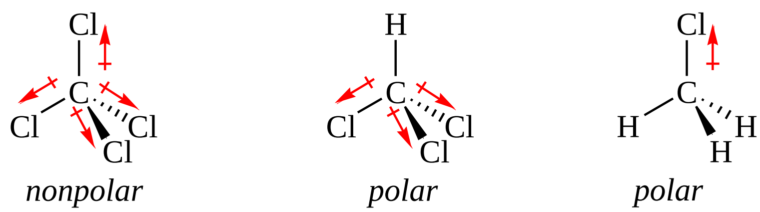
For example, consider the Lewis dot structure for carbon dioxide. This is a linear molecule, containing two polar carbon-oxygen double bonds. However, since the polar bonds are pointing exactly 180° away from each other, the bond polarities cancel out, and the molecule is nonpolar. (As an analogy, you can think of this is being like a game of tug of war between two teams that are pulling on a rope equally hard.)

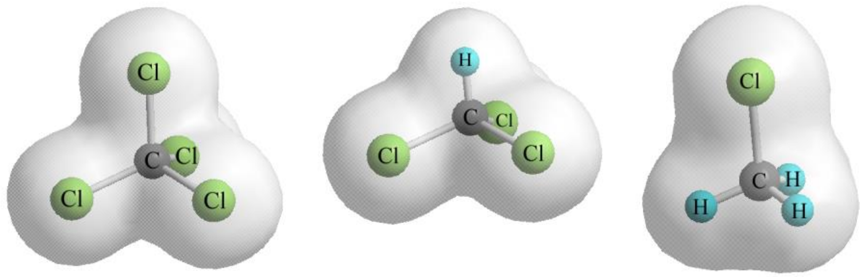


The water molecule also contains polar bonds, but since it is a bent molecule, the bonds are at an angle to each other of about 105°. They do *not* cancel out because they are not pointing exactly towards each other, and there is an overall dipole going from the hydrogen end of the molecule towards the oxygen end of the molecule; water is therefore a polar molecule:



Molecules in which all of the atoms surrounding the central atom are the same tend to be nonpolar if there are no lone pairs on the central atom. If some of the atoms surrounding the central atom are different, however, the molecule may be polar. For example, carbon tetrachloride, CCl_4, is nonpolar, but chloroform, $CHCl_3$, and methyl chloride, CH_3Cl are polar:





The polarity of a molecule has a strong effect on its physical properties. Molecules which are more polar have stronger intermolecular forces between them (dipole-dipole and H-bonding), and have, in general, higher boiling points (as well as other different physical properties).

Examples

Methane (CH_4)

Carbon Dioxide (CO_2)

Putting it all Together

Examples

Phosgene ($COCl_2$)

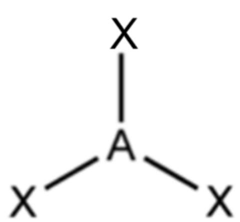
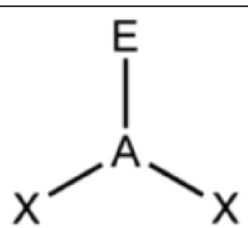
Ethanol (CH_3CH_2OH)

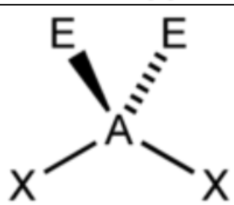
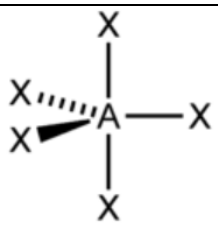
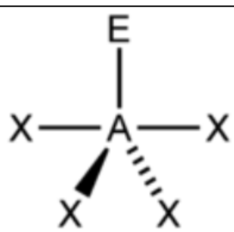
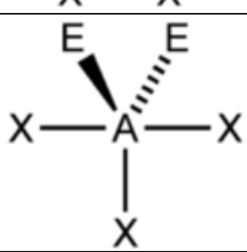
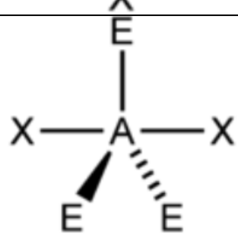
2.3 Assignment/Lab Activity

Grab your molecular model kit and build the following molecules to help you fill in the table below. You will have blank boxes as some molecular shapes are much more common than others.

H_2O	PCl_5
BF_3	SF_6
XeF_4	N_2O
H_3O^+	XeF_2
HCN	SF_4
ClF_3	CH_3F
NO	O_3

Note, this table utilized the AXE method. "A" is the central atom. "X" are the bonded atoms (peripheral atoms). "E" if the unbound/lone pairs of electrons.

Shape	# Bonding Pair(s)	#Lone electron pairs	Molecular Geometry	Example **Specify whether your example is polar of nonpolar
				
				
				
				

Shape	# Bonding Pair(s)	#Lone electron pairs	Molecular Geometry	Example **Specify whether your example is polar of nonpolar
				
				
				
				
				
				
				

Shape	# Bonding Pair(s)	#Lone electron pairs	Molecular Geometry	Example **Specify whether your example is polar of nonpolar