Chemistry 120 Fall 2016

Instructor: Dr. Upali Siriwardane

e-mail: upali@latech.edu
Office: CTH 311
Phone 257-4941

Office Hours: M,W,F 9:30-11:30 am T,R 8:00-10:00 am or by appointment;

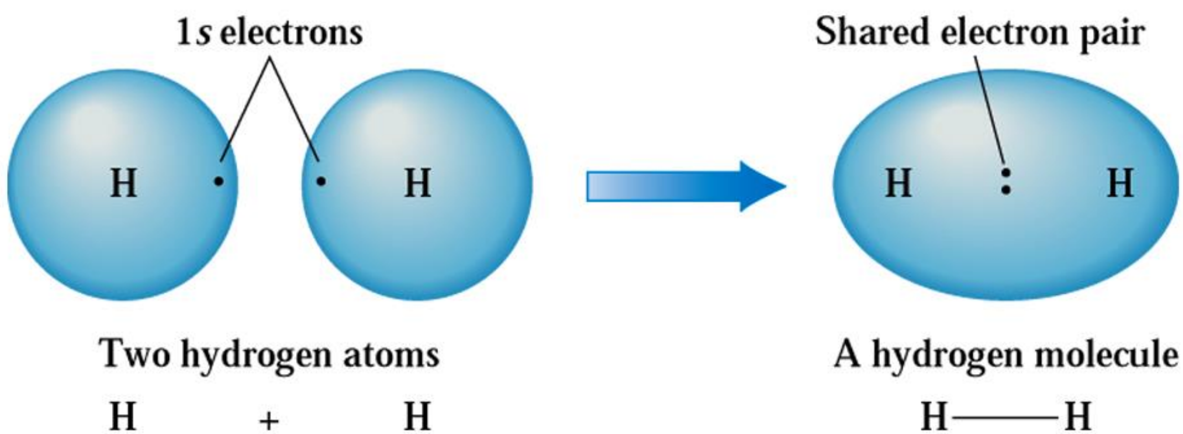
Test Dates:

September 23, **2016 (Test 1): Chapter 1,2 &3**
October 13, **2016 (Test 2): Chapter 4 & 5**
October 31, **2016 (Test 3): Chapter 6, 7 & 8**
November 15, **2016 (Test 4): Chapter 9, 10 & 11**
November 17, **2016 (Make-up test) comprehensive: Chapters 1-11**

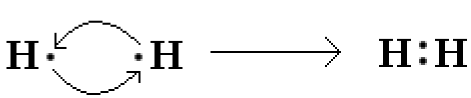
Chapter 5. Chemical Bonding: The Covalent Bond Model

The covalent bond model

- Covalent bonds result from the sharing of electrons between atoms. These electron pairs (bonds) act like a glue to hold atoms together.

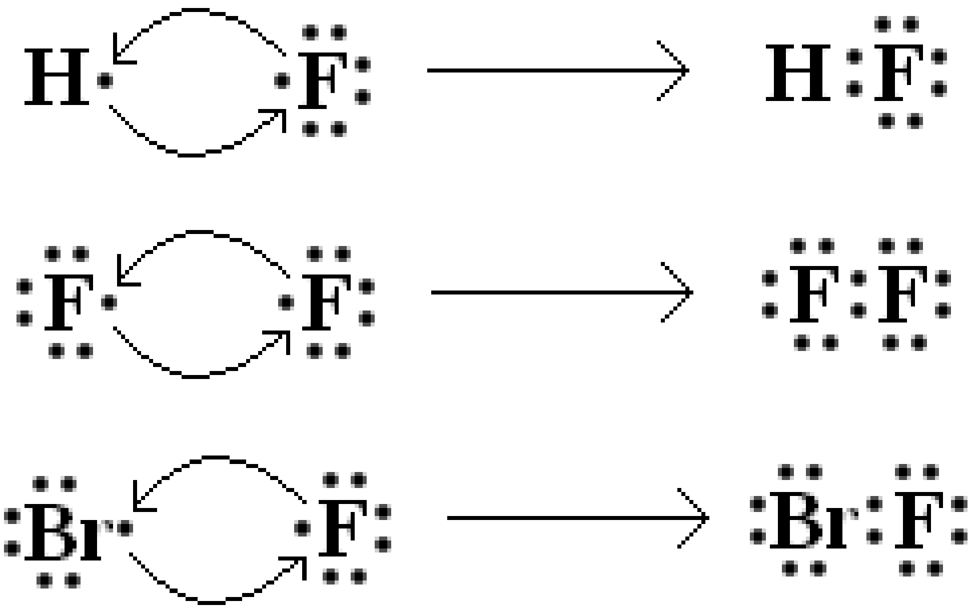


Covalent bonds result between hydrogen atoms when the 1s orbitals of two atoms overlap

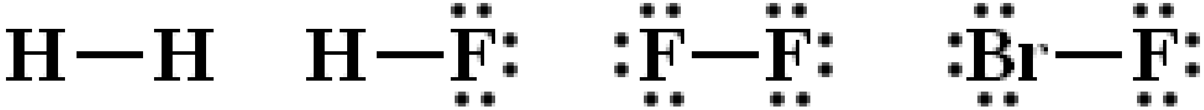


in Lewis notation

Lewis structures for molecular compounds

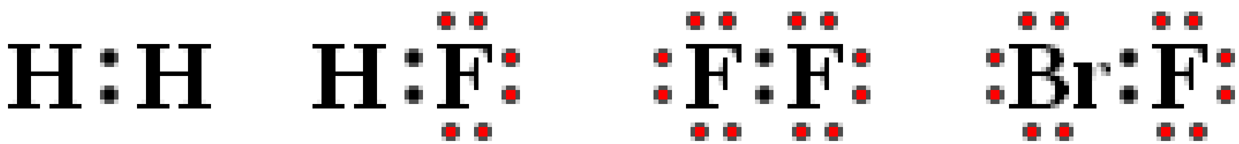


Usually, we represent shared electron pairs with lines (1 line = 1 covalent bond)



When counting electrons around an atom in Lewis structures, each covalent bond counts as 2 electrons

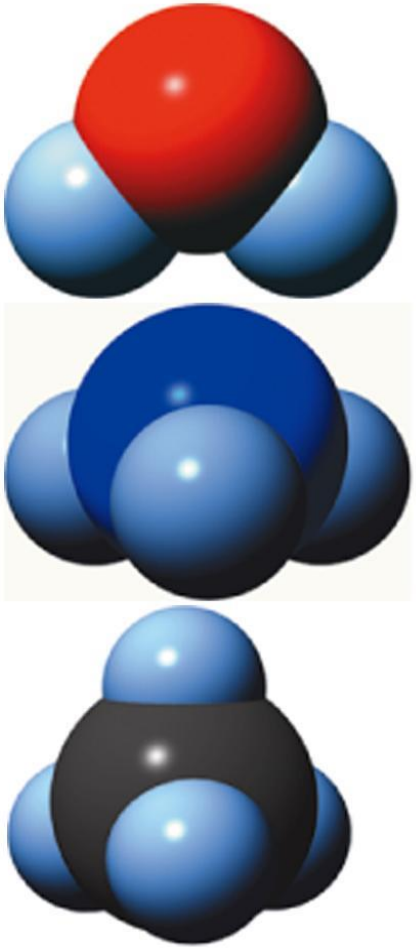
Lewis structures for molecular compounds

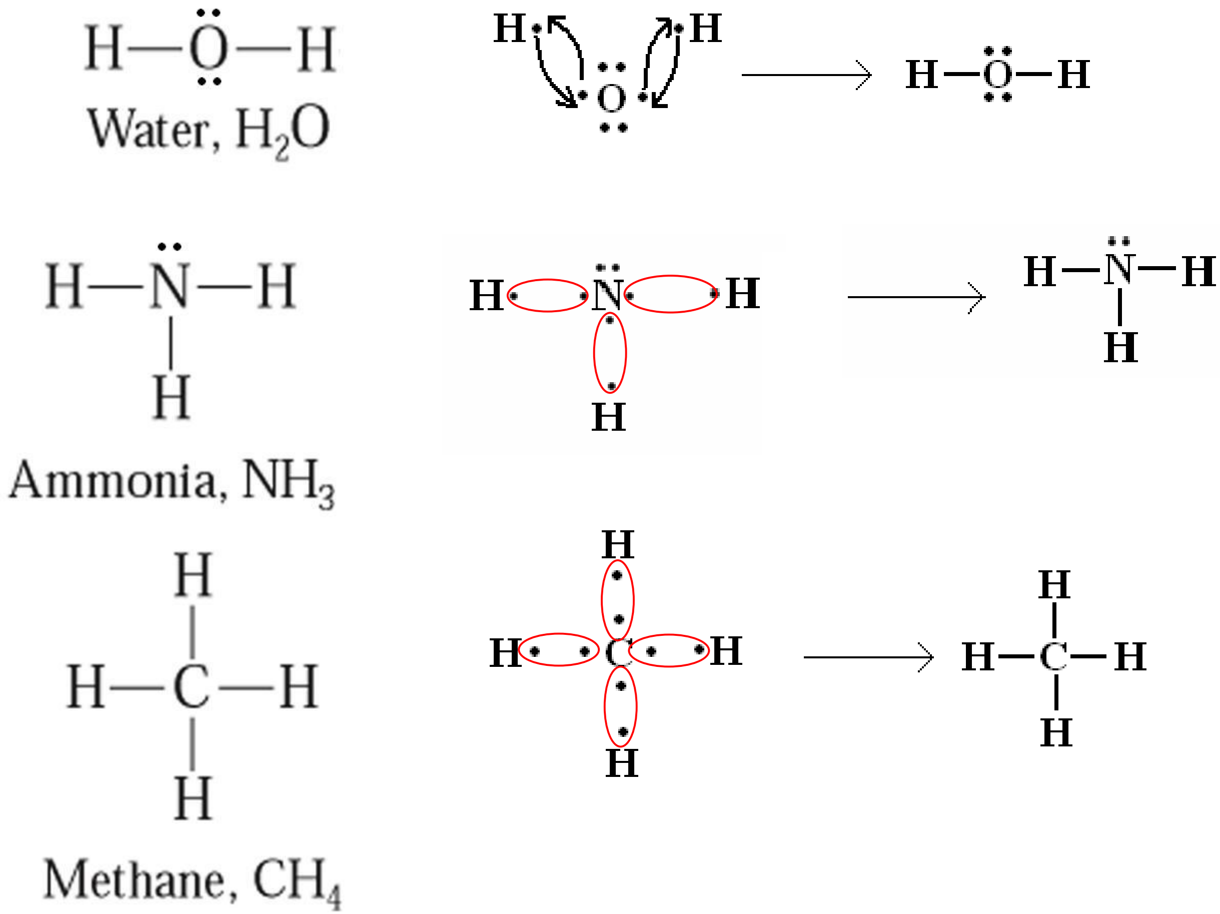


Electrons that aren’t involved in bonds are called “non-bonding electrons” (labeled in red in the above diagrams)

Lewis structures for molecular compounds

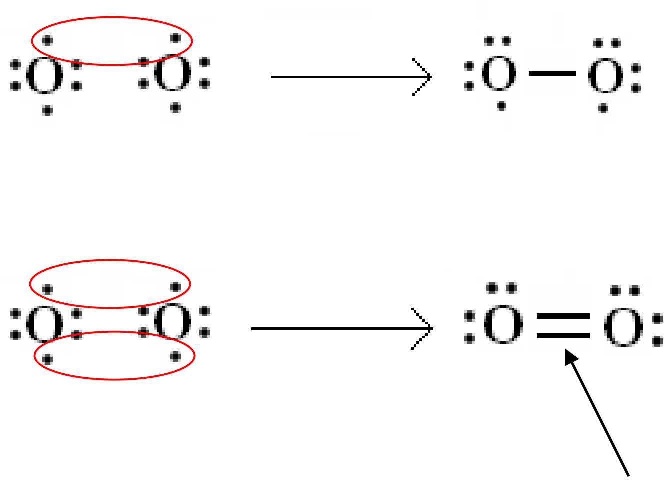
Lewis structures are not meant to convey anything about shape





Single, double, and triple covalent bonds

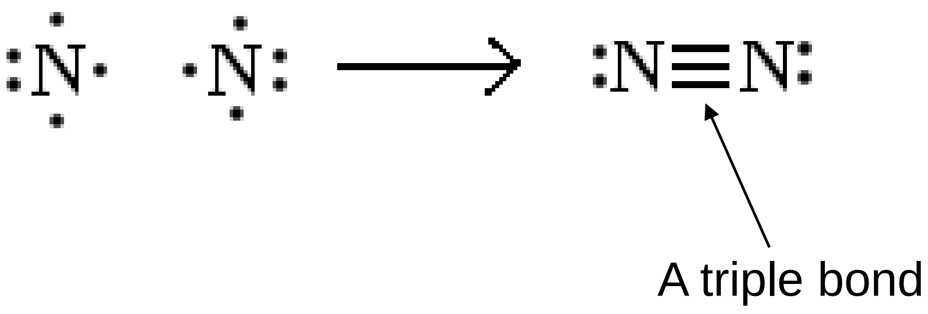
- In single bonds, atoms share a pair of electrons; the electron pair that is shared exists in the space between the two atoms' nuclei.
- In certain cases, atoms must share *more* than just a pair of electrons to explain the bonding between them. For example, in O_2, sharing just one pair leaves each oxygen atom with only 7 electrons around it…but sharing another pair gives each of them 8 electrons.



This is called a double covalent bond

Single, double, and triple covalent bonds

- Another example is N_2 (nitrogen). In this case, two N atoms need to share three pairs of electrons for each N atom to gain an octet.

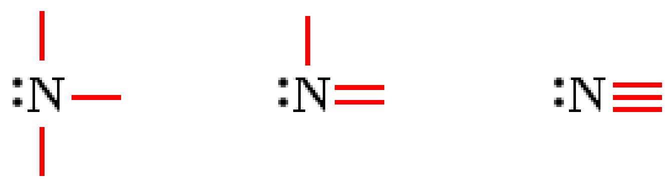


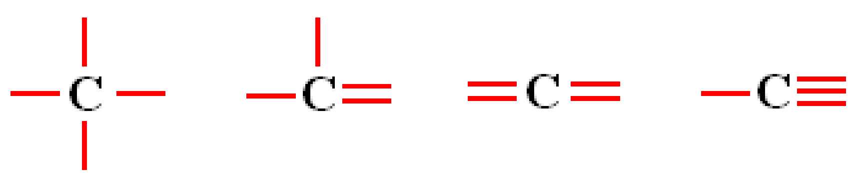
Valence electrons and the number of covalent bonds formed

- To predict how many bonds an atom will form to obtain an octet, consider the number of valence electrons it possesses.

Oxygen: group 6A; needs
to form two bonds to get octet

Nitrogen: group 5A; needs
to form three bonds to get octet





Carbon: group 4A; needs
to form four bonds to get octet

	1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	8B 9	8B 10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18
1	1 **H**																	2 **He**
2	3 **Li**	4 **Be**											5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
3	11 **Na**	12 **Mg**											13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
4	19 **K**	20 **Ca**	21 **Sc**	22 **Ti**	23 **V**	24 **Cr**	25 **Mn**	26 **Fe**	27 **Co**	28 **Ni**	29 **Cu**	30 **Zn**	31 **Ga**	32 **Ge**	33 **As**	34 **Se**	35 **Br**	36 **Kr**
5	37 **Rb**	38 **Sr**	39 **Y**	40 **Zr**	41 **Nb**	42 **Mo**	43 **Tc**	44 **Ru**	45 **Rh**	46 **Pd**	47 **Ag**	48 **Cd**	49 **In**	50 **Sn**	51 **Sb**	52 **Te**	53 **I**	54 **Xe**
6	55 **Cs**	56 **Ba**	71 **Lu**	72 **Hf**	73 **Ta**	74 **W**	75 **Re**	76 **Os**	77 **Ir**	78 **Pt**	79 **Au**	80 **Hg**	81 **Tl**	82 **Pb**	83 **Bi**	84 **Po**	85 **At**	86 **Rn**
7	87 **Fr**	88 **Ra**	103 **Lr**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110	111	112	113	114	115	116		

57 **La**	58 **Ce**	59 **Pr**	60 **Nd**	61 **Pm**	62 **Sm**	63 **Eu**	64 **Gd**	65 **Tb**	66 **Dy**	67 **Ho**	68 **Er**	69 **Tm**	70 **Yb**
89 **Ac**	90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**

Metals

Metalloids

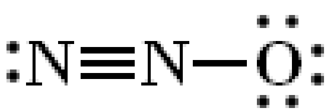
Nonmetals

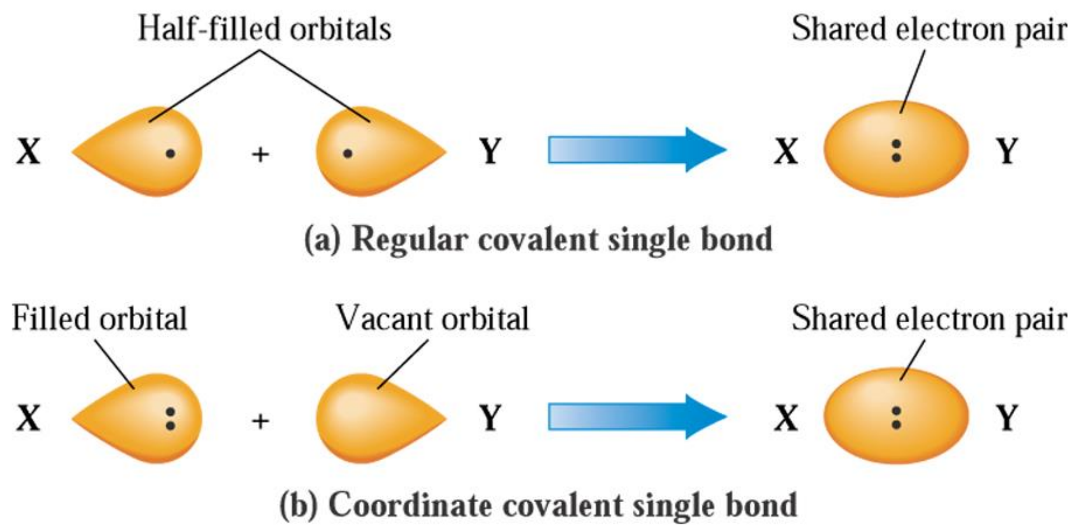
Coordinate covalent bonds

- In some cases, atoms may donate both electrons that are used to form a bond. Examples:

- CO 

- N_2O





Systematic rules for drawing Lewis structures

- Step 1: Find the sum of valence electrons of all atoms in the polyatomic ion or molecule.
- Step 2: Draw the atoms in the order in which they occur*, connecting them with single bonds. Bonds "cost" 2 electrons each.
- Step 3: Add electrons around the non-central (outside) atoms until they each have an octet.**
- Step 4: If any electrons remain left over at this point, use them to complete the octet on the central atom.

*See page 115 to predict which atom is central in a formula. Neither hydrogen nor fluorine is *ever* a central atom. If C is present, it usually is the central atom, and in binary compounds (e.g. NH_3), the "single-atom element" is usually the central atom.
** Remember, hydrogen atoms can accommodate only 2 electrons (i.e. not an octet).

Systematic rules for drawing Lewis structures

- Step 5: If there are not enough electrons on the central atom for an octet, make multiple bonds between the central atom and another atom to give it an octet.
- Step 6: Double-check the total number of electrons in the Lewis structure at this point to be sure that there are no more present than the total number you counted in Step 1.

- Examples: SO_2, HCN, CO_2

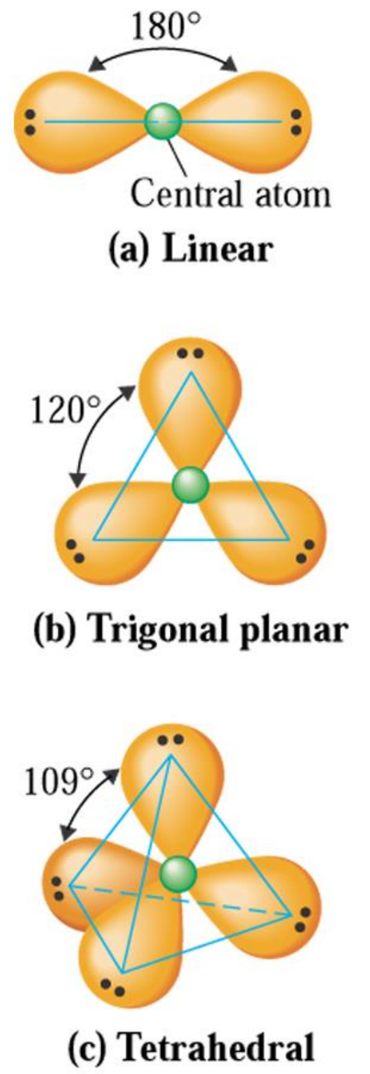
Bonding in polyatomic ions and ionic compounds containing polyatomic ions

- The rules for drawing Lewis structures for polyatomic ions are similar to the six steps we just covered.
- Ions carry charges, so the total number of electrons calculated in Step 1 must be adjusted to account for the ion's charge.
  - Positive charged ions: deduct one electron from the total number counted for each positive charge.
  - Negatively charged ions: add one electron to the total number for each negative charge.
  - In the end, surround the Lewis structure with square brackets and indicate charge as for Lewis structures for ionic compounds

Examples: SO_4^{2-},K_2SO_4, CO_3^{2-}

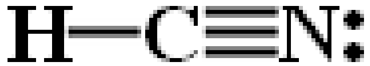
VSEPR theory

- Looking at a Lewis structure, one might expect that all molecules are flat; Lewis structures convey no information (by themselves) about the shape of molecules.
- VSEPR theory (Valence Shell Electron-Pair Repulsion) is used to predict molecular shape, and is based on the repulsion that exists between charges of the same sign.
- Shape of a molecule is normally given with respect to the central atom.



VSEPR theory

- Consider the electron pairs that are found on the central atom in a molecule of HCN

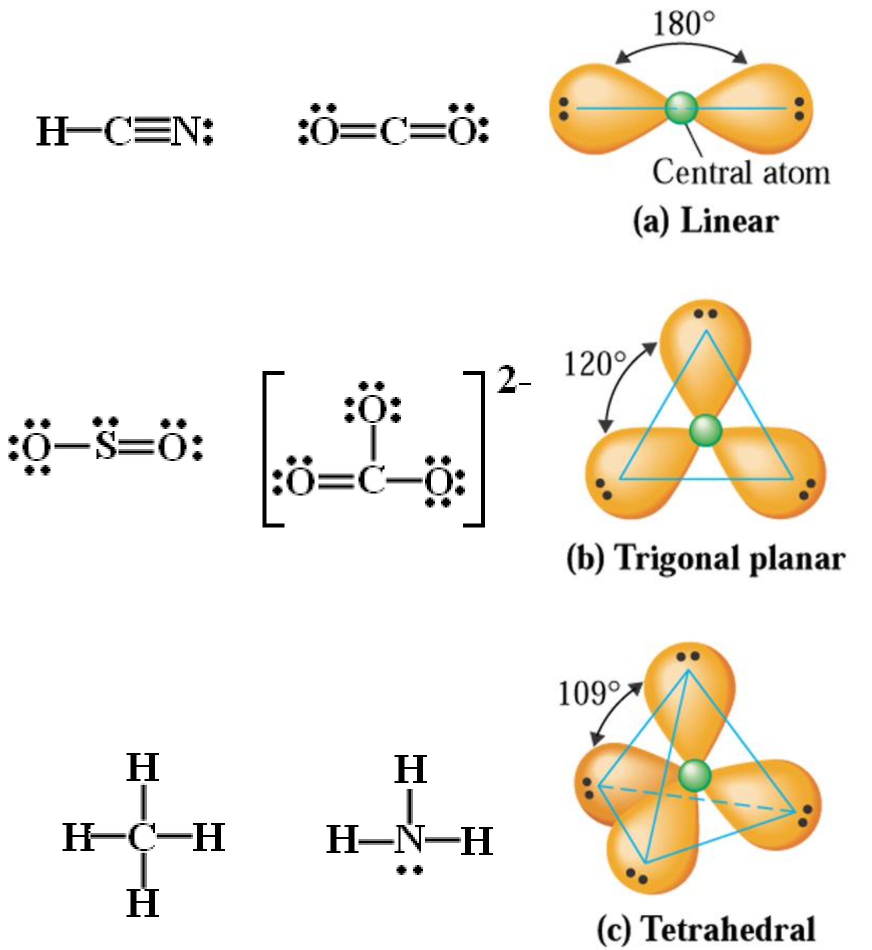


- On one side of the central carbon atom is a C-H single bond, and on the other, a C-N triple bond. Thus, there are two “VSER electron groups” around the carbon.
- These bonds consist of electrons, and are repulsive toward each other. The bonds prefer to be as far apart from each other as possible, yielding a linear arrangement.

VSEPR electron groups = single bond, double bond, triple bond, or a non-bonding pair of electrons (all are negatively charged)

VSEPR theory

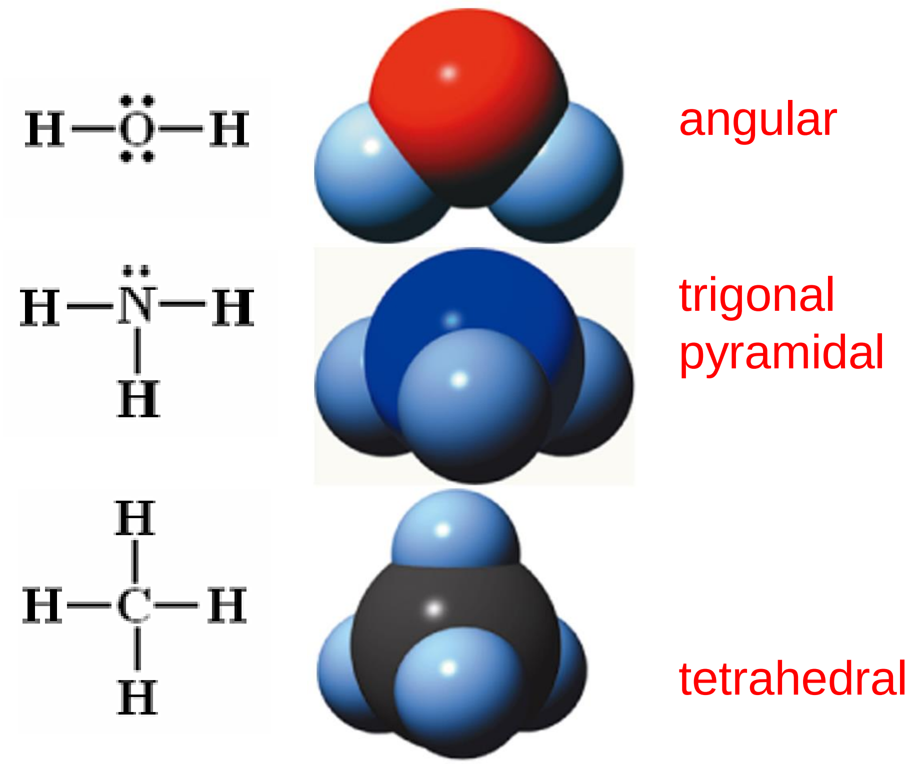
- The number of VSEPR electron groups on the central atom is what determines the structure's geometry. As these groups are repelled by each other, and move as far apart as they can, they drag with them the outer atoms.
- Two VSEPR electron groups on the central atom yields a linear arrangement of these electron groups.
- Three VSEPR electron groups yields a trigonal planar arrangement of electron groups.
- Four VSEPR electron groups on the central atom yields a tetrahedral arrangement of electron groups.



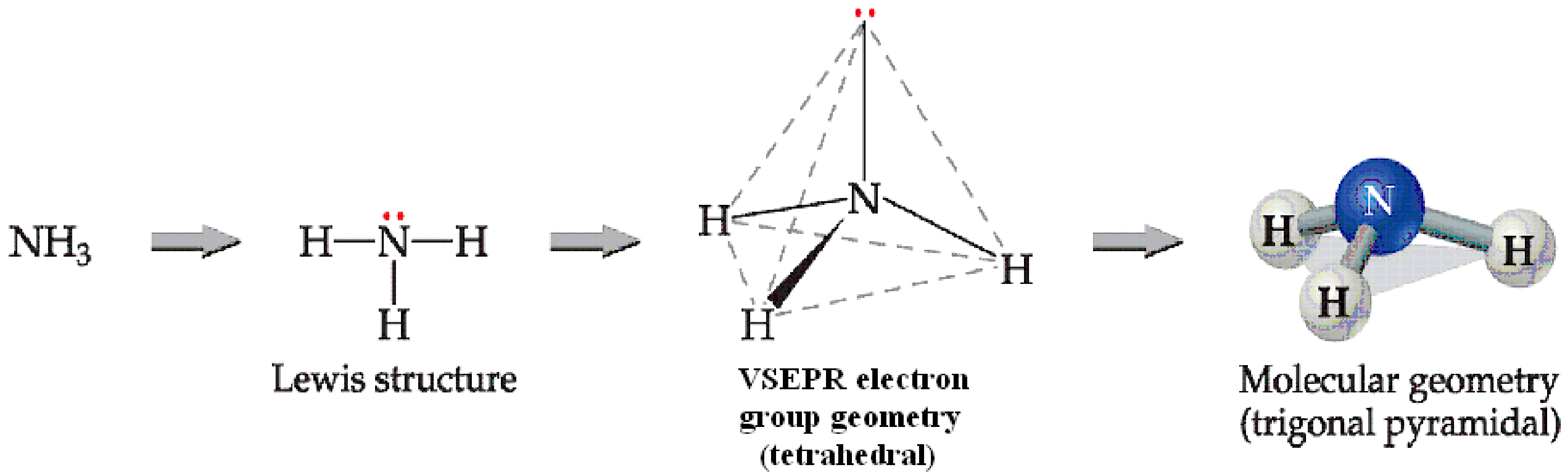
VSEPR theory

All of these Lewis structures have four electron domains on the central atom

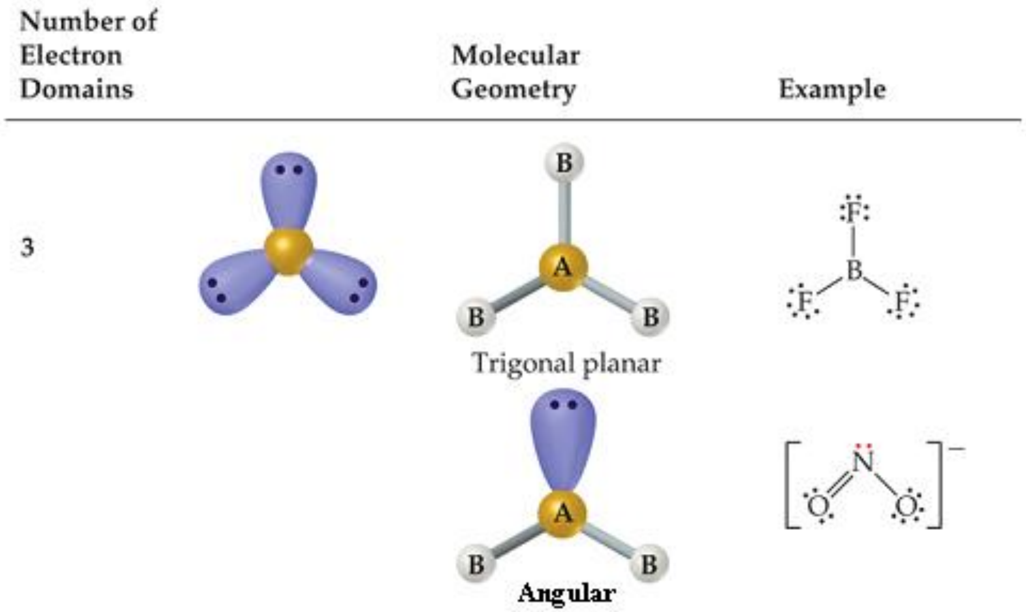
- In many cases, at least one of the VSEPR electron groups on the central atom is a non-bonding pair.
- The shape of the molecule is determined by the arrangement of *atoms* around the central atom.



VSEPR theory



VSEPR theory



- There are two molecular geometries for 3 electron domains:
  - Trigonal planar, if all the electron domains are bonding
  - Angular, if one of the domains is a nonbonding pair.

Examples: CO_3^{2-}, O_3, NO_2^-

PREDICTING MOLECULAR GEOMETRY USING VSEPR THEORY

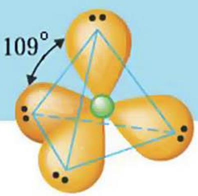
Operational rules

1. Draw a Lewis structure for the molecule.
2. Count the number of VSEPR electron groups about the central atom in the Lewis structure.
3. Assign a geometry based on minimizing repulsions between electron groups.

VSEPR ELECTRON GROUP ARRANGEMENTS	MAKEUP OF VSEPR GROUPS	MOLECULAR GEOMETRY
Tetrahedral	4 bonding	Tetrahedral
	3 bonding 1 nonbonding	Trigonal pyramid
	2 bonding 2 nonbonding	Angular
Trigonal Planar	3 bonding	Trigonal planar
	2 bonding 1 nonbonding	Angular
Linear	2 bonding	Linear

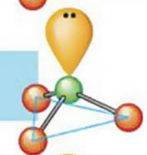
Tetrahedral

Occurs when four VSEPR electron groups are present about a central atom

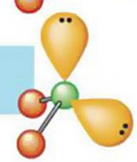


- 4 bonding → Tetrahedral

- 3 bonding, 1 nonbonding → Trigonal pyramid

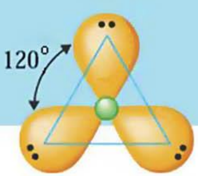


- 2 bonding, 2 nonbonding → Angular

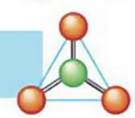


Trigonal Planar

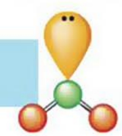
Occurs when three VSEPR electron groups are present about a central atom



- 3 bonding → Trigonal planar

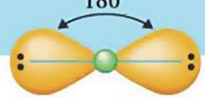


- 2 bonding, 1 nonbonding → Angular

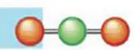


Linear

Occurs when two VSEPR electron groups are present about a central atom

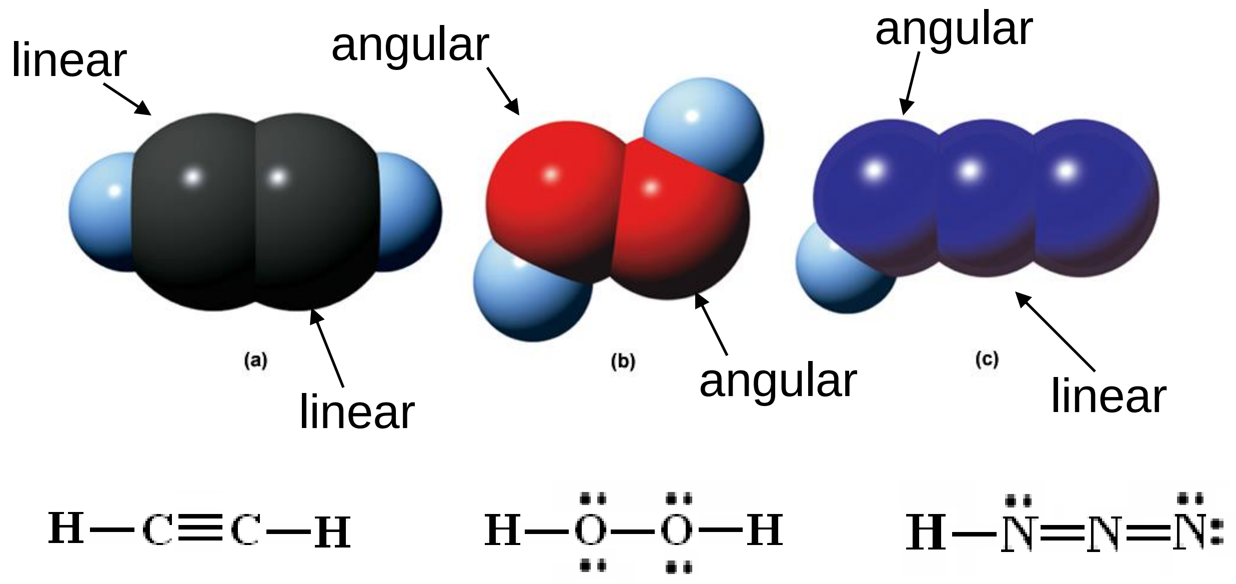


- 2 bonding → Linear



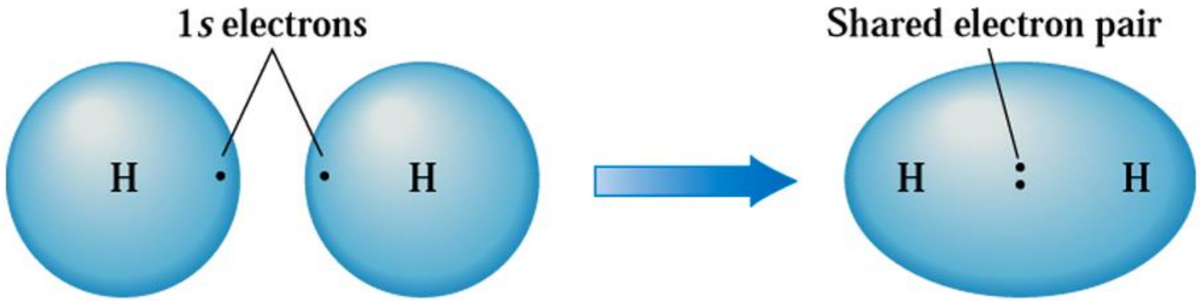
Molecules with more than one central atom

- For molecules that contain more than one central atom, a local molecular shape can be described (describing the geometry around a central atom).



Electronegativity

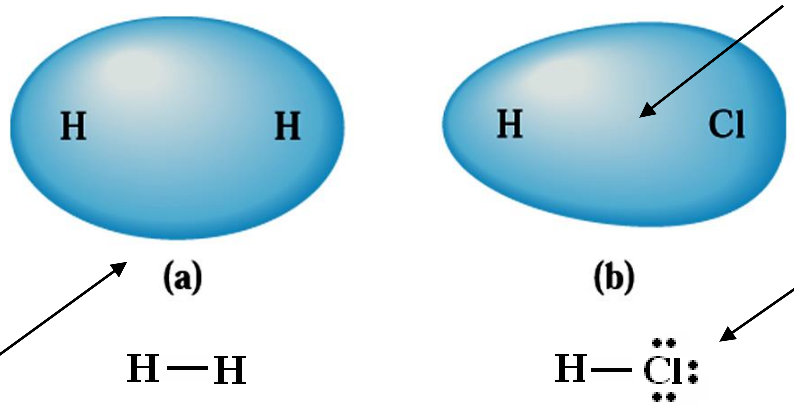
- Atoms that are involved in bonds share electron with other atoms to obtain octet of electrons around themselves.
- When two identical atoms share electrons to form bonds, the electrons in the bond(s) are shared equally between the two atoms (e.g. H_2, O_2, N_2, and between the two carbon atoms of C_2H_2 – see last slide).



Electronegativity

- In many covalent bonds, the electron pair (or pairs, in multiple bonds) are not equally shared, as different elements have differing abilities to attract electrons <u>in bonds</u> toward themselves.
- The electronegativity of an element reflects how strongly an atom of that element can pull *bonding* electrons toward itself.

This bond is called a <u>polar covalent bond</u>

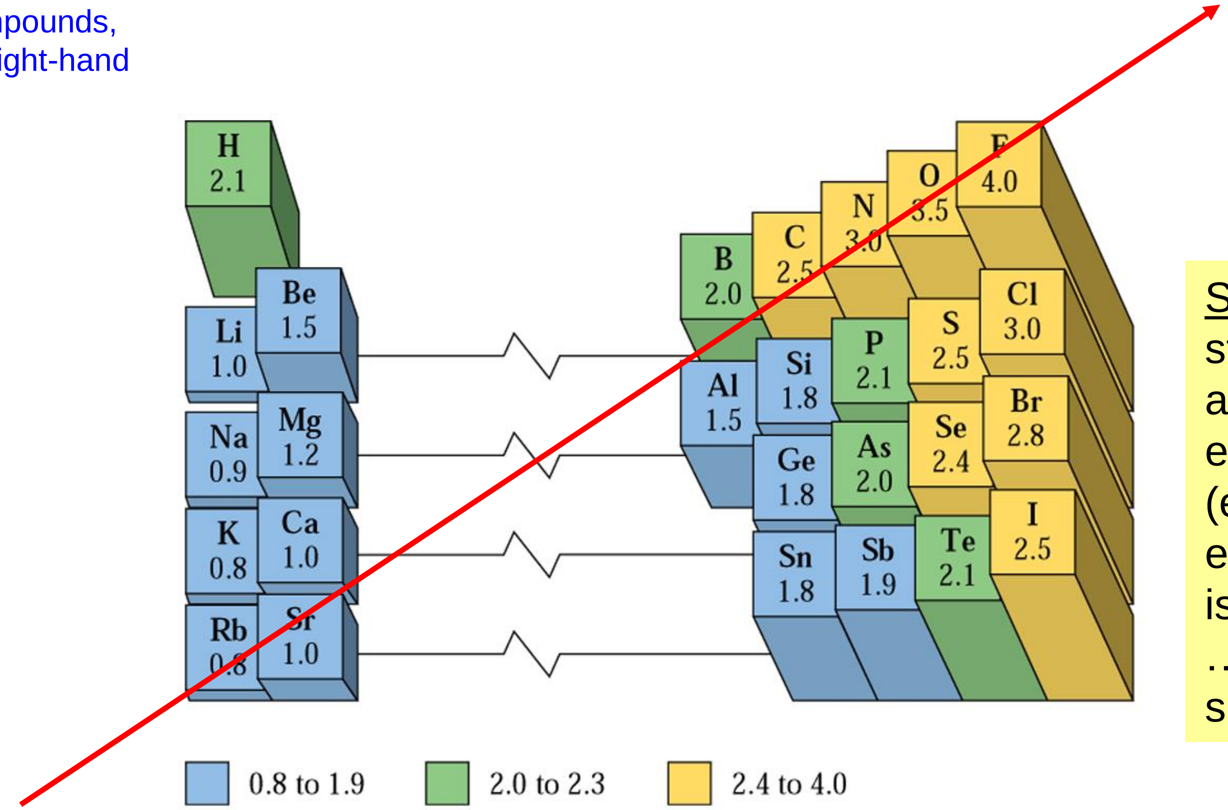


Chlorine is more electronegative than hydrogen, so the electrons in the H-Cl bond spend more time near Cl than H

This bond is a <u>non-polar covalent bond</u>

Electronegativity

Consistent with the idea that elements on the left-hand side of the periodic table lose electrons in forming ionic compounds, while those on the right-hand side gain electrons

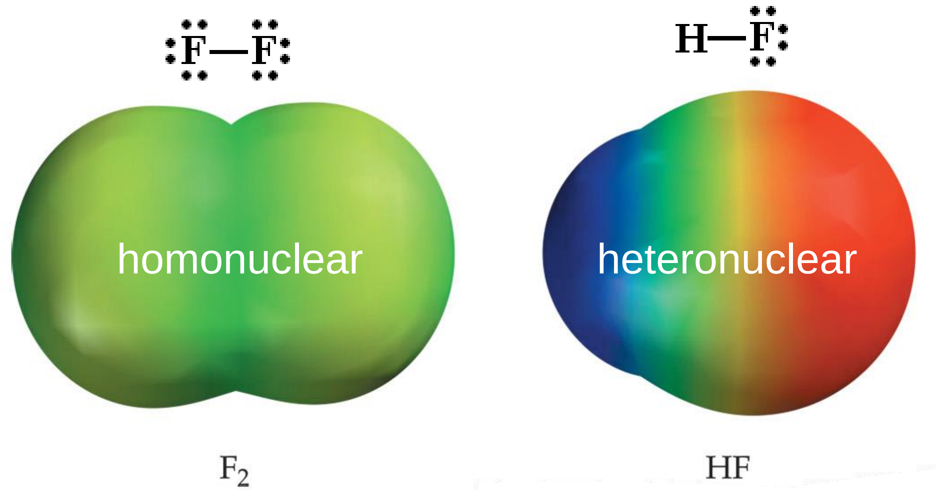


<u>Sidebar</u>: in a Lewis structure, the central atom is the least electronegative atom (except if the least electronegative atom is hydrogen) …remember N_2O on slide 10

Electronegativity increases left-to-right across a period and bottom-to-top in a group.

Bond polarity

- Polar covalent bonds have an unsymmetrical distribution of electrons between the two atoms involved in the bond.
- The electrons in these bonds spend more time on one side of the bond (the side with the more electronegative atom) than the other.
- This creates a bonding picture that looks a *bit* like an ionic bond; however, no electron transfer has happened here (electrons are still shared, just unequally).



Non-polar covalent bond
Polar covalent bond

The bigger the difference in the electronegativity of the two atoms in the covalent bond, <u>the more polar the bond</u>.

Bond polarity

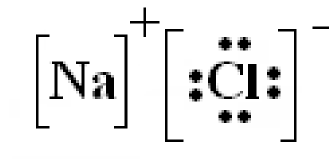
- Polar bonds are somewhere in-between non-polar covalent bonds and ionic bonds

Non-polar covalent

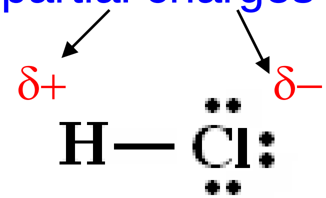
Equal sharing of electrons in bonds

Ionic bonds

Complete transfer of electron(s) from one atom to the other (no sharing)



partial charges

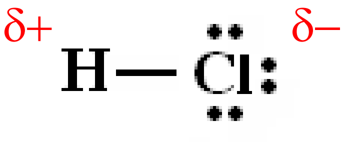


Polar covalent bonds

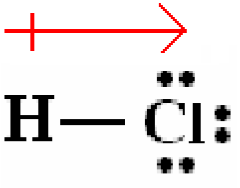
Unequal sharing of bonding electrons; endows one end of bond with partial negative charge and the other with a partial positive charge

Bond polarity

- Because the bonding electrons between H and Cl spend more time on the Cl end, that end of the bond carries a partial negative charge (and the other end a partial positive charge)



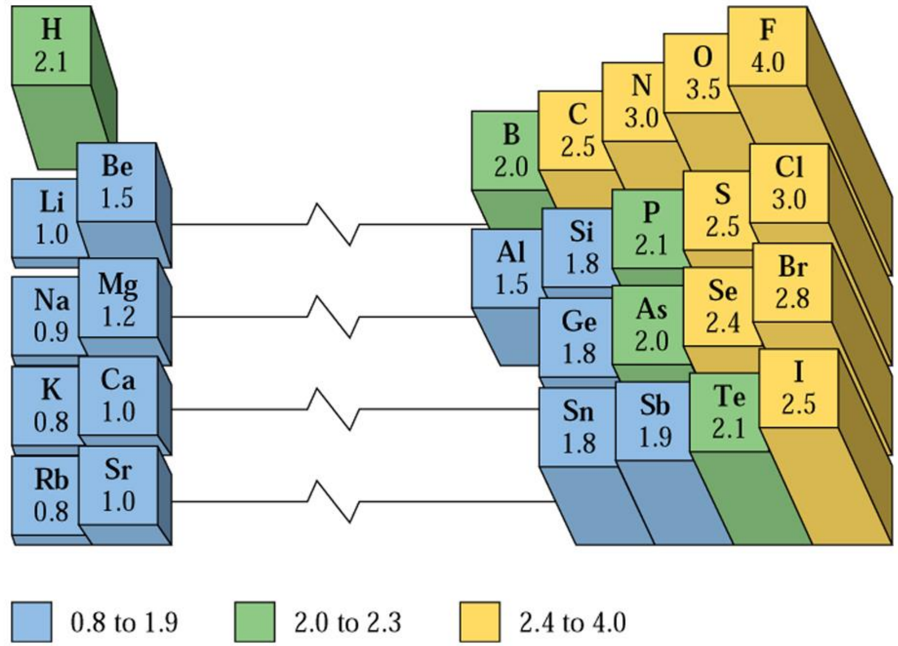
- This can also be represented with a "crossed arrow"



- In this notation, the arrow points toward side of the bond that carries the partial negative charge and the "+" sign is on the side that carries the partial positive charge.

Bond polarity

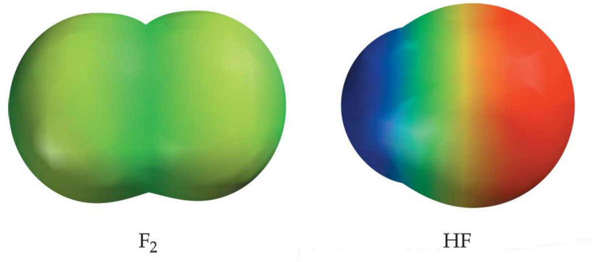
- In some cases, bonds that have low polarity are considered to be non-polar.
- Use the following guideline to determine whether a bond is non-polar, polar, or ionic:
  - If the two atoms involved in a bond have an electronegativity difference of 0.4 or less, the bond is considered to be non-polar covalent.
  - If the electronegativity difference for the two atoms of a bond is between 0.4 and 1.5, it is considered to be a polar covalent bond.
  - Bonds that have an electronegativity difference of greater than 2.0 are ionic.
  - If the electronegativity difference for a bond lies in the 1.5-2.0 range, it is considered to be ionic if it involves a metal and non-metal. It is considered to be polar covalent if two non-metals are involved



H-H	non-polar covalent
C-H	non-polar covalent
H-Cl	polar covalent
H-F	polar covalent
Na-Cl	ionic

Molecular polarity

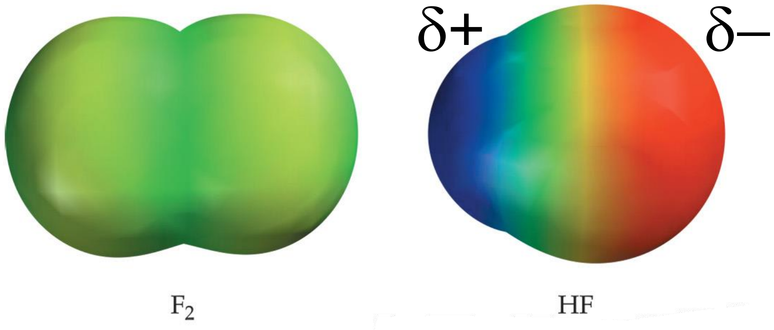
- Entire molecules can have unequal distributions of electronic charge. In these cases, the molecule is said to be polar.
- An easy-to-see case for this is in a H-F molecule. The bond is polar and there is only one bond in the molecule. Thus the entire molecule is polar.
- Molecules may be polar as a result of a combination of
  - their molecular geometry
  - the presence of polar bonds in the molecule



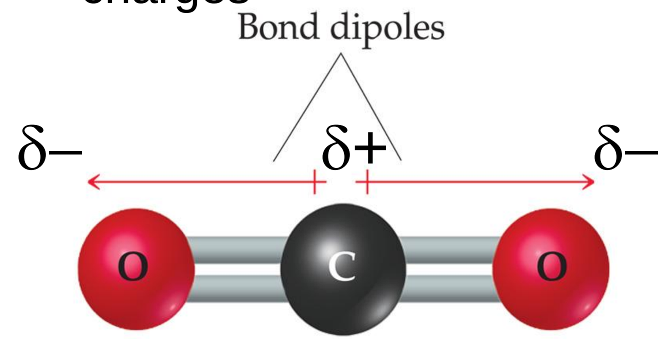
Molecular polarity

non-polar covalent

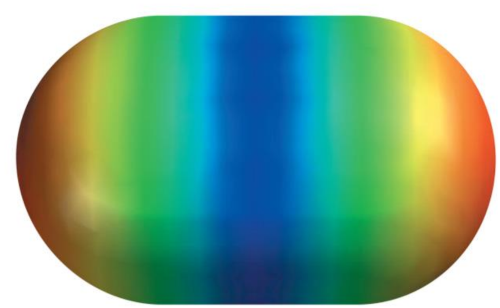
polar covalent



“partial” charges

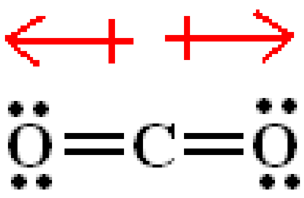


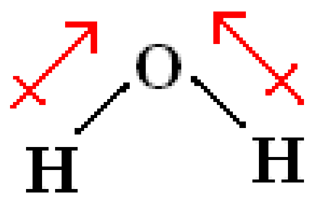
- Just because a molecule possesses polar bonds does not mean the molecule *as a whole* will be polar.



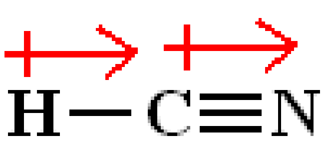
Molecular polarity

- Unlike CO_2 (triatomic, linear, and symmetric), H_2O is not linear (angular), and so the direction of its polar bonds describes an H_2O molecule that has a partial negative charge on the oxygen side, and a partial positive charge on the hydrogen side.



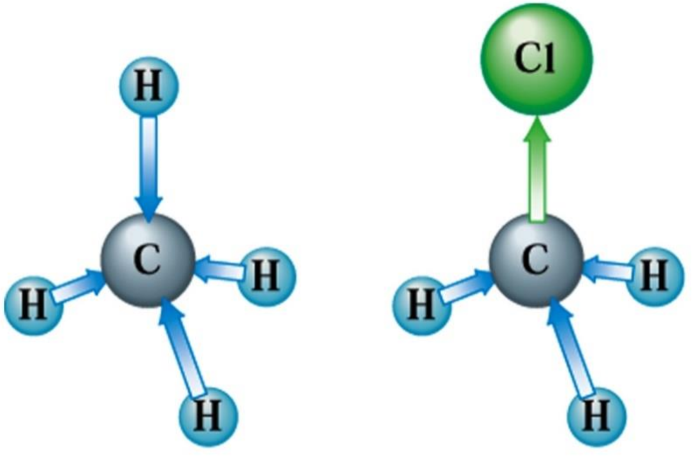


- For HCN, it is easier to see why the molecule is polar



Molecular polarity

- For more complicated molecules (e.g. CH_4, CH_3Cl), the symmetry of the molecule needs to be considered to predict whether the molecule is polar or not.



(a) Methane (b) Methyl chloride

Naming binary molecular compounds

- Binary molecular compounds contain only two non-metallic elements.
- In naming binary molecular compounds, the non-metal of lower electronegativity is presented first, followed by the non-metal having the higher electronegativity. The non-metal's name is suffixed as it was for binary ionic compounds ("-ide").
  - HF: hydrogen fluoride
- For compounds with more than one atom of an element, prefixes are used to indicate the numbers of these atoms*:
  - N_2O_4: dinitrogen tetroxide
  - NO_2: nitrogen dioxide

Exception: if the first element is hydrogen , then the prefix is not used.
Example, H_2S is just "hydrogen sulfide"