

## Chapter 1:

# Review of Atomic Structure, Chemical Bonding, and Lewis Structures

“Big things have small beginnings, sir.”  
– Mr. Dryden (Claude Rains) in film *Lawrence of Arabia*

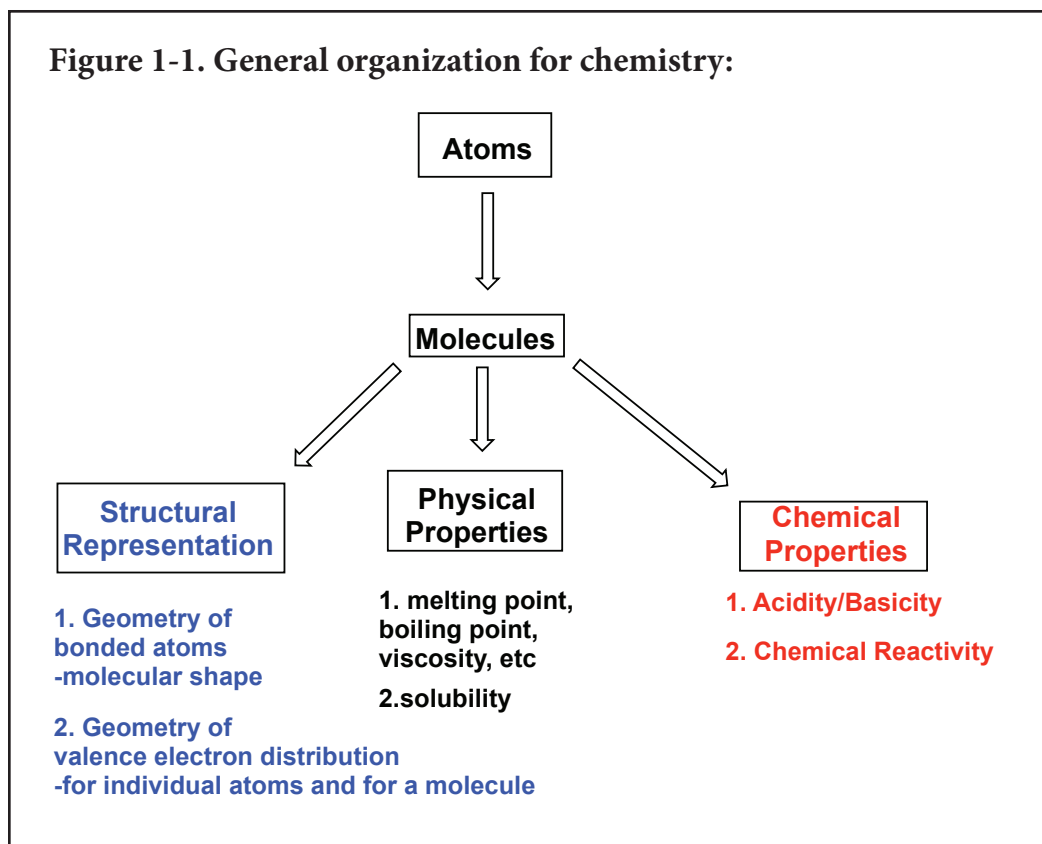
### 1-1. Introduction:

No matter how complex a molecular structure, it still is composed of atoms. Each of those atoms in that molecule contributes their valence electrons and their atomic properties to that structure. Thus to understand molecular structure and its affect on chemical reactivity, you'll need to at least have some superficial understanding of atomic structure.

### 1-2. What will be presented:

1. What are the components of atomic structure important to chemistry?
2. How are the electron clouds around atoms organized?
3. What are the four quantum numbers?
4. What is described by each of those quantum numbers?
5. What is an electron configuration?
6. How are ground state electron configurations determined?
7. What is the relationship between electron configurations and the Mendeleev Periodic Table?
8. What drives the formation of chemical bonds?
9. What are the types of chemical bonds?
10. What is the difference between an ionic bond and a polar covalent bond?
11. What is a bond dipole?
12. How do you draw Lewis structures for simple molecules?
13. What is formal charge and how is it determined?
14. What is an oxidation number and how is it determined?

**Figure 1-1. General organization for chemistry:**



The structure of this text will be to build upward and outward — from atoms to first form simple molecules — and then to form more complex molecules. Atoms bind to other atoms to form molecules and most of the chemistry that will be discussed here is predicated on the idea that it is molecular structure that affects both chemical and physical properties.

It also is important to understand that chemical reactions and reactivity are built up from some rather simple ideas relating changes in bonding to changes in energy. One of the most important of these “simple” ideas is the connection between Lewis acid-base interactions and chemical reactivity. Most of the chemistry discussed here will be treated, as much as possible, as an extension of Lewis acid-base chemistry.

What follows in the remaining sections of Ch 1 is a very quick review of General Chemistry topics about atomic structure that are essential to readers as they begin to study Organic Chemistry. These topics are summaries of basic concepts and components used to describe atomic structure, the organization of the Periodic Table, and the formation of simple molecules. These same ideas also will be used to facilitate our understanding of molecular electronic structure and the chemistry of more complex molecules.

### 1-3. Components of a nuclear atom:

Rutherford's famous gold foil experiment determined that an atom was nuclear in its structure. *Nuclear* means that more than 99% of an atom's mass can be found in its nucleus. Those atomic components of general interest to chemistry are the *proton*, the *neutron*, and the *electron*. The numbers of protons in a nucleus, an atom's atomic number, defines an element. Each proton has a charge of +1. Neutrons are the electrical insulators in a nucleus and do not have any charge. The number of neutrons in a nucleus is always equal to or greater than the number of protons in that nucleus. Electrons form the outer electrical "cloud" that surrounds an atom's nucleus. Each electron has a charge of -1 and a mass that is about 1/1837th that of a proton.

**Table 1-1. Atomic components and properties:**

Particle	Charge*	Mass(amu)	Location in atom
Proton	+1	1.0073	Component of Nucleus
Neutron	0	1.0087	Component of Nucleus
Electron	-1	0.00055	Outside of Nucleus

\* relative to charge on a proton, actual charge is  $1.602 \times 10^{-19}$  coulomb

**For an uncharged or neutral atom:**

1. number of  $e^-$  = number of protons
2. number of neutrons is either equal to or greater than the number of protons

Each element has its own unique one or two letter designation. At a minimum, atomic representation typically consists of specifying which element, the number of times it appears within a molecular formula, and the amount of charge, if any, on that atom or a group of atoms:

**Figure 1-2. Information provided by atomic representations:**

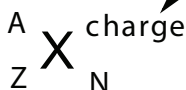
Quadrants around atomic symbol (i.e. X) are used to provide additional information about that element

A: is a mass number used designate a specific isotope of element X

Charge refers to charge on atom X. can be + or -

Z: Atomic number; number of protons for element X, see in nuclear chemistry. normally this designation is redundant

N: number of atoms of atom X in molecular structure or fragment



Most of Organic Chemistry utilizes the main group elements shown below. You are responsible for knowing the symbols for those main group elements colored in blue:

**Figure 1-3. Summary of Main Group elements important to Organic Chemistry:**

1A									Noble Gases
H	2A						He		
Li	Be	3A	4A	5A	6A	7A	Ne		
Na	Mg	Al	Si	P	S	Cl	Ar		
K	Ca	1B	2B	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Cu	Zn	In	Sn	Sb	Te	I	Xe
Cs	Ba	Ag	Cd	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Au	Hg						

## 1-4. Organization of the electron cloud surrounding an atomic nucleus:

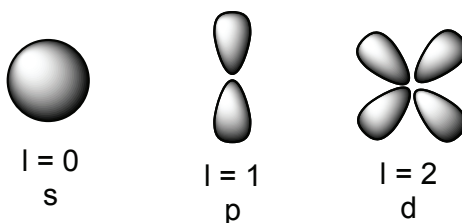
Subsequent spectroscopic investigations revealed that the electron cloud surrounding a nucleus was organized — initially it was thought to be like a mini solar system. In the period from about 1920 to 1930, this Bohr model for an atom's electron structure was replaced by the wave model. This new model instead describes the electron cloud surrounding a nucleus in terms of spherical standing waves of electrons. These standing waves of electrons are characterized by four quantum numbers:

**Figure 1-4. The four quantum numbers necessary for describing the states of electrons bound to atoms:**

### Quantum Numbers for atomic electrons: $n$ , $l$ , $M_l$ and $M_s$ or $S$

**$n$**  -The principle quantum number. Values for  $n$  begin at 1-the first and closest orbital to a nucleus. The principle quantum number increases as one moves farther away from a nucleus;  $n = 1, 2, 3, 4, \dots$

**$l$** : Angular momentum or Azimuthal quantum number. Values for  $l$  range from 0 to  $n-1$ . This is the quantum number that specifies the shape of an orbital (s, p, d, or f):



**$M_l$**  -The magnetic or orientation quantum number. There are  $2l+1$  possible values for  $M_l$  of a given angular quantum number- $l$ .

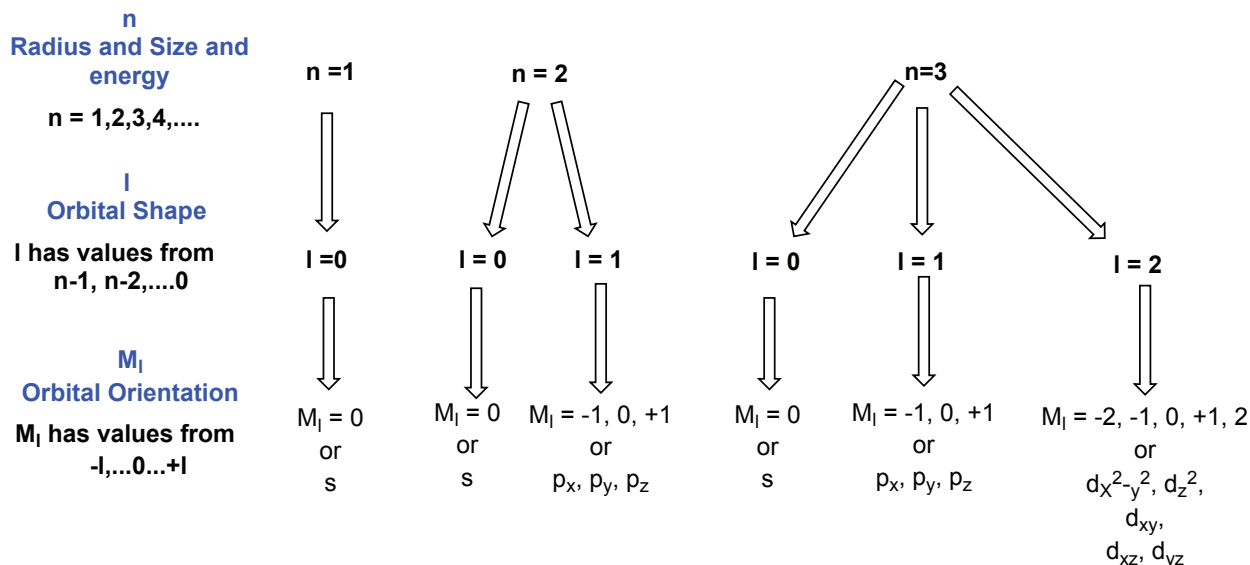
Possible values for  $M_l$  range from:  $-l, -(l-1), \dots, 0, \dots, 1, 2, \dots, +l$

This quantum number specifies the possible orientations for a given orbital shape. e.g.  $P_x, P_y, P_z$

**$M_s$**  -Spin quantum number.  $M_s$  has two possible values  $+1/2$  or  $-1/2$

Figure 1-5 below shows how two of these quantum numbers are dependent on the value of the principle quantum numbers  $l$  and  $M_l$  are ( $n$ ):

**Hierarchy of Quantum numbers (the value of  $n$  determines  $l$  and  $M_l$ ):**



The only quantum number, not dependent on the value of the principle quantum number (i.e.  $n$ ) is electron spin (i.e.  $M_s$ ). An electron only can have a spin of  $+$  or  $- \frac{1}{2}$  (i.e.  $M_s = +1/2$  or  $-1/2$ ).

Any electron bound to any atom may be characterized in terms of these four quantum numbers. A complete listing of all occupied orbitals surrounding an atom is known as an atom's *electron configuration*. A proper, lowest energy, electron configuration for any atom must comply with three rules:

**Aufbau Principle:** One fills atomic orbitals from the lowest value of  $n$  to the highest value of  $n$  possible for the number of electrons under consideration.

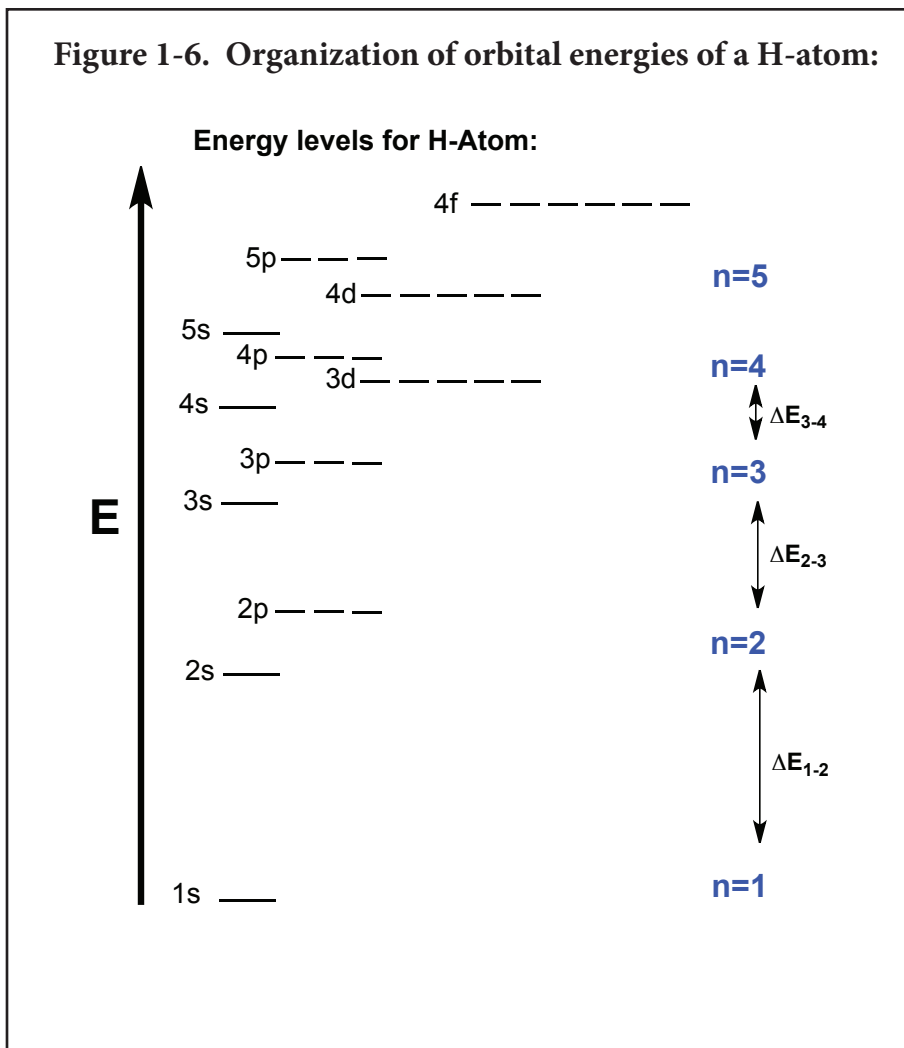
**Pauli exclusion Principle:** Each electron must have a unique set of quantum numbers. As a practical matter it is this principle that limits the maximum number of electrons that occupy any orbital to only 2 electrons.

**Hund's Rule of Maximum multiplicity:** Orbitals of equal energy are occupied, first by a single electron before a second electron of opposite spin is added to fill that orbital.

These are the rules used to construct the most stable electron configuration of an atom. This most stable electron configuration is referred to as an atom's *ground state* or *ground state electron configuration*.

Possible atomic energy levels based on the electronic structure of an H-atom look like that shown in Figure 1-6:

**Figure 1-6. Organization of orbital energies of a H-atom:**



Notice that the farther one moves outward or away from a nucleus, the greater the value of  $n$  (i.e. the principle quantum number), and the lower the value of its orbital energies (i.e. or alternatively, the lower the ionization energy for an electron in that higher orbital energy level). However, also notice that the energy spacings between sequential values of  $n$  also decrease with increasing values of  $n$ :

**Eq. 1-1:**

$$\Delta E(n=1s \text{ to } n=2s) \gg \Delta E(2s-3s) \gg \Delta E(3s-4s) \gg \Delta E(4s-5s)$$

As a principle quantum number ( $n$ ) increases, there also are increases in both the number of possible orbital shapes and orbital orientations for those shapes. Notice that as the separation between successive levels become smaller, the bands of orbital energies begin to interpenetrate each other. Starting at  $n=3$ , its 3d orbital energy is at a higher orbital energy than is its  $n=4$ , 4s orbital.

**Q: If  $n=3$  and the magnetic quantum number ( $l$ ) =2, then what is the orbital shape?**

**Ans:** d-orbital shape

**Q: Which sets of quantum numbers cannot occur?**

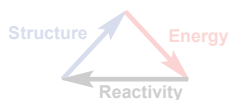
n	l	m <sub>l</sub>	Exist?
1	1	1	No
2	0	-1	No
3	2	2	Yes
2	1	0	Yes

Elements with similar valence electron configurations are the organizational basis of Mendeleev's Periodic Table. It's not the entire complete electron configurations of an element that are important, rather it's an element's valence electron configurations that are crucial in determining an atom's chemical and physical properties. *Valence electrons* refers to those electrons occupying the outer most energy levels of an atom's electron configuration (i.e. those occupied orbitals with largest values of n). Typically chemically reactive elements possess electron configurations that consist of incompletely filled valence orbitals.

**Figure 1-7. Valence electron configurations for the Main Group elements:**

1A							Noble Gases				
H	2A			3A	4A	5A	6A	7A	He		
H 1s <sup>1</sup>									He 1s <sup>2</sup>		
Li [He]2s <sup>1</sup>	Be [He]2s <sup>2</sup>		[He]	B 2s <sup>2</sup> 2p <sup>1</sup>	C 2s <sup>2</sup> 2p <sup>2</sup>	N 2s <sup>2</sup> 2p <sup>3</sup>	O 2s <sup>2</sup> 2p <sup>4</sup>	F 2s <sup>2</sup> 2p <sup>5</sup>	Ne 2s <sup>2</sup> 2p <sup>6</sup>		
Na [Ne]3s <sup>1</sup>	Mg [Ne]3s <sup>2</sup>		[Ne]	Al 3s <sup>2</sup> 3p <sup>1</sup>	Si 3s <sup>2</sup> 3p <sup>2</sup>	P 3s <sup>2</sup> 3p <sup>3</sup>	S 3s <sup>2</sup> 3p <sup>4</sup>	Cl 3s <sup>2</sup> 3p <sup>5</sup>	Ar 3s <sup>2</sup> 3p <sup>6</sup>		
K [Ar]4s <sup>1</sup>	Ca [Ar]4s <sup>2</sup>		[Ar]	1B Cu 4s <sup>1</sup>	2B Zn 4s <sup>2</sup>	Ga 4s <sup>2</sup> 4p <sup>1</sup>	Ge 4s <sup>2</sup> 4p <sup>2</sup>	As 4s <sup>2</sup> 4p <sup>3</sup>	Se 4s <sup>2</sup> 4p <sup>4</sup>	Br 4s <sup>2</sup> 4p <sup>5</sup>	Kr 4s <sup>2</sup> 4p <sup>6</sup>
Rb [Ar]5s <sup>1</sup>	Sr [Ar]5s <sup>2</sup>		[Kr]	Ag 5s <sup>1</sup>	Cd 5s <sup>2</sup>	In 5s <sup>2</sup> 5p <sup>1</sup>	Sn 5s <sup>2</sup> 5p <sup>2</sup>	Sb 5s <sup>2</sup> 5p <sup>3</sup>	Te 5s <sup>2</sup> 5p <sup>4</sup>	I 5s <sup>2</sup> 5p <sup>5</sup>	Xe 5s <sup>2</sup> 5p <sup>6</sup>
Cs [Xe]6s <sup>1</sup>	Ba [Xe]6s <sup>2</sup>		[Xe]	Au 6s <sup>1</sup>	Hg 6s <sup>2</sup>	Tl 6s <sup>2</sup> 6p <sup>1</sup>	Pb 6s <sup>2</sup> 6p <sup>2</sup>	Bi 6s <sup>2</sup> 6p <sup>3</sup>	Po 6s <sup>2</sup> 6p <sup>4</sup>	At 6s <sup>2</sup> 6p <sup>5</sup>	Rn 6s <sup>2</sup> 6p <sup>6</sup>
Fr [Rn]7s <sup>1</sup>	Ra [Rn]7s <sup>2</sup>		[Rn]								

\*\* Note that this table above uses the old group numbering system. These old group numbers are useful because they correspond to the number of valence electrons present for those atoms that belong to that group or family of elements. This will be useful when we consider molecule formation and Lewis Structures.





For Mendeleev's Periodic Table, elements within a group have same number of valence electron or valence electron configurations. This is illustrated above for the Main Groups of elements, which contain both metals and non-metals important to Organic Chemistry.

**Q: What is the complete ground state electron configuration for Nitrogen?**

Ans:  $1s^2 2s^2 2p^3$

**Q: What is the expected ground state electron configuration for  $\text{Si}^{-1}$  (Silicon has an atomic number of 14 and a -1 negative charge)? How many valence electrons for an  $\text{Si}^{-3}$  ion?**

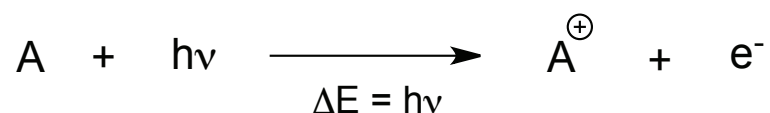
Ans:  $1s^2 2s^2 2p^3 3s^2 3p^3$  for  $\text{Si}^{-3}$ :  $4 + 3 = 7$

**Q: What is the expected electronic configuration stability for the series of Ge anions:  $\text{Ge}^{-2}$ ,  $\text{Ge}^{-1}$  and  $\text{Ge}^{-4}$ ? Why would you expect this particular sequence?**

Ans: Order of stability is:  $\text{Ge}^{-4} > \text{Ge}^{-2} > \text{Ge}^{-1}$  because  $\text{Ge}^{-4}$  is closer to a Kr electron configuration than are  $\text{Ge}^{-2}$  and  $\text{Ge}^{-1}$ .

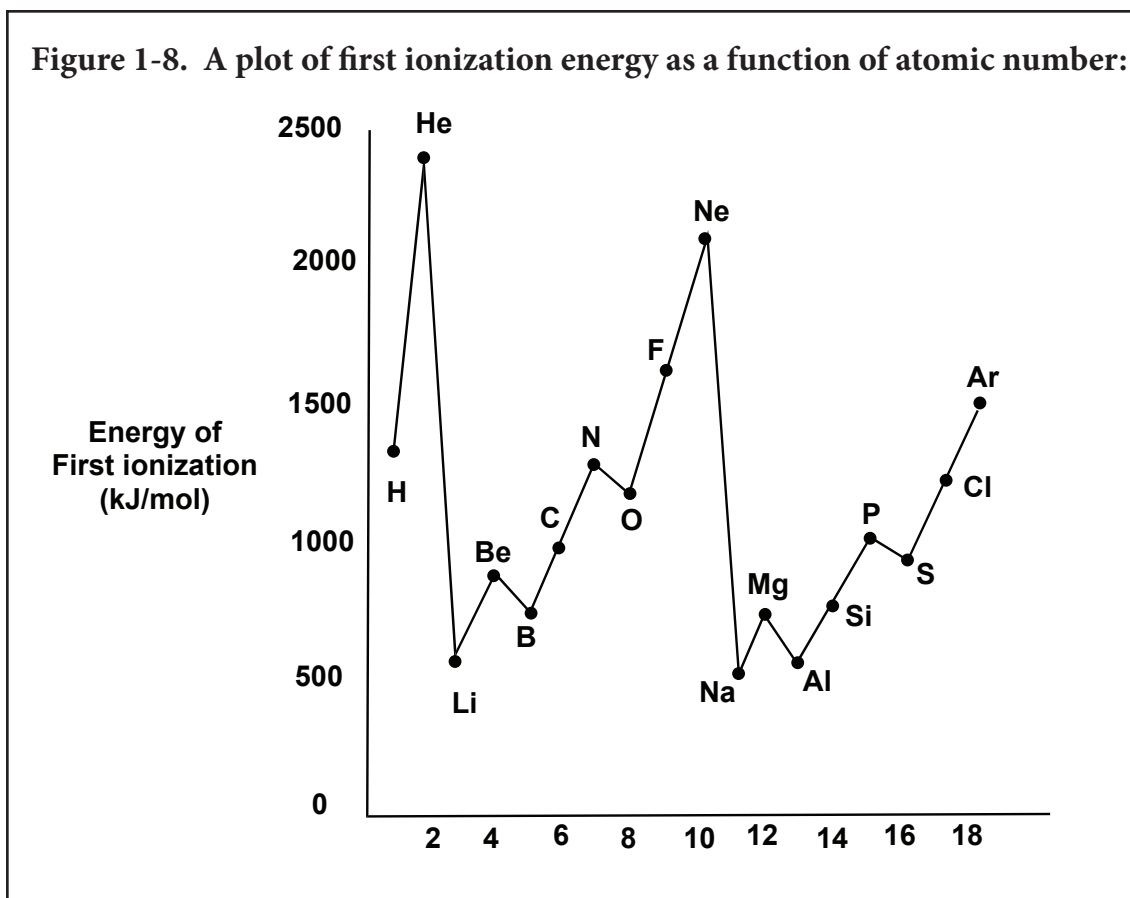
*Electronegativity* (EN) is an atomic property that reflects the tendency of an atom to pull electron density to itself within a covalent chemical bond. The values of electronegativity (EN) increase as one moves from left to right across a row of the Periodic Table. The larger the value of an atom's EN, the smaller an atom's radius. Also the larger the value of EN for an atom, the greater the amount of energy required for ionization. Ionization energy is the minimum energy (i.e.  $h\nu$ ) required to pull an electron from an atom (A) to form a cation ( $\text{A}^+$ ) and a free unbound electron ( $\text{e}^-$ ):

Eq. 1-2:



The graph below plots the increasing amounts of energy required to remove one valence electron from an atom as a function of atomic number. Ionization energy increases steadily as one proceeds across a row from a Group 1 element, on the left of a row, to a Noble Gas (Group 8) element, on the right of that row. Figure 1-8 is perhaps one of the more dramatic demonstrations of the stability provided by the complete valence electron octets (i.e.  $ns^2 np^6$ ) of the Noble gases.

Figure 1-8. A plot of first ionization energy as a function of atomic number:



This saw-tooth structure of Fig. 1-8 is most dramatic for elements of the first and second rows of the periodic table. Notice that the Noble Gasses have the highest ionization energies of any element in their respective row of the periodic table (e.g. He has a more stable electron configuration than H).

For atoms within molecules, the stability of an atom's atomic electron configuration also affects an atom's pull on its share of covalently bonded electron density. This "pull" can be assessed by Pauling's electronegativity scale. Pauling's Electronegativity values (i.e. EN) for the main group elements are shown in Fig. 1-9:

**Figure 1-9. Tabulation of Pauling's electronegativity (EN) values for the Main Group elements:**

1A		2A		3A		4A		5A		6A		7A		Noble Gases
H 2.1														He ----
Li 1.0	Be 1.5			B 2.0	C 2.5	N 3.0	O 3.5	F 4.0						Ne ----
Na 0.9	Mg 1.2			Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0						Ar ----
K 0.8	Ca 1.0	1B	2B											
Rb 0.8	Sr 1.0	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8						Kr ----
Cs 0.7	Ba 0.9	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5						Xe ----
Fr 0.7	Ra 0.9	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2						Rn ----

**Q: Why is the EN for B greater than the EN of Be?**

**Ans:** Be is an element closer to the He electron configuration than it is to a Ne electron configuration. As a result, Be is more likely to give up two electrons to attain an He configuration than it is to gain six electrons in an effort to attain a Ne configuration. Thus in its covalent bonding Be who's atomic electron will be much less electronegative and more likely to form Be<sup>+2</sup>, than say, another non-metal like B who's electron configuration is closer to Ne than to He.

### 1-5. Bonds and Bonding:

The reason atoms form chemical bonds is to attain Noble Gas electron configurations. It is this drive to complete their valence orbital octets that is the basis of all chemistry.

#### A Review of Bond Types:

**Metallic Bonding-** Metallic bonds have positive metal cations surrounded by a "sea" of freely mobile valence electrons that are delocalized over very large numbers of these metallic atoms. Such "delocalized" bonding (i.e. bonding that is distributed or spread between more than two atoms) produces both high electrical and thermal conductivities for these metallic materials. This delocalized bonding is what makes metals not only good electrical conductors but also mechanically malleable and ductile.

**Ionic Bonding** — Ionic bonds are formed when valence electrons are transferred from a more electron rich donor (i.e. electropositive) atom onto a more electron deficient acceptor (i.e. electronegative) atom. This electron transfer simultaneously creates positive and negatively charged ions. Ionic compounds tend to form high melting crystalline solids that also will conduct electricity when in their molten states.

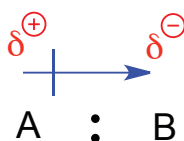
Ionic bonds are easy to understand — valence electrons are transferred from one atom to another atom. The transfer of electrons between atoms is driven by formation of ions with Noble Gas like electron configurations.

**Covalent Bonding** — Covalent bonding occurs when valence electrons are shared between atoms. Types of covalent bonds include both *non-polar* and *polar covalent bonds*. Within a non-polar covalent bond, these bonding electrons are shared equally between the two bonded atoms.

For polar covalent bonds, one of the bonded atoms, as a result of its larger electronegativity, exerts a stronger pull on this shared electron density. This stronger pull results in an unequal sharing of bonded electrons and creates some partial ionic character that adds to the strength of this type of covalent bond. As a result of this unequal sharing of bonded electrons, the less electronegative (i.e. more electropositive) atom, that partially donates some of its electron density acquires a slight positive charge relative to the more electronegative acceptor atom at the other end of this bond that acquires a slight negative charge:

**Figure 1-10. Formation of bond dipoles from polar covalent bonds:**

**Bond dipole for A-B:**



**EN(B) > EN(A)**

⇨ as the bonding e<sup>-</sup> pair is pulled closer to B, it creates partial ionic charges at the ends of the A-B bonding axis. Thus dipole arrow points at the partially negatively charged B atom .

A polar covalent bond occurs anytime there are two different elements covalently bonded to each other (e.g. heteronuclear A-B (single), or A=B (double), or even A≡B (triple) covalent bonds). The only true non-polar covalent bonds are formed between atoms of the same element (i.e. homonuclear covalent bonds).

**Q: For an ionic bond, the atom that loses e<sup>-</sup> becomes a \_\_\_\_\_ ion**

**Ans: cation or cationic**

**Q: The atom that gains electrons in an ionic bond becomes a \_\_\_\_\_ ion.**

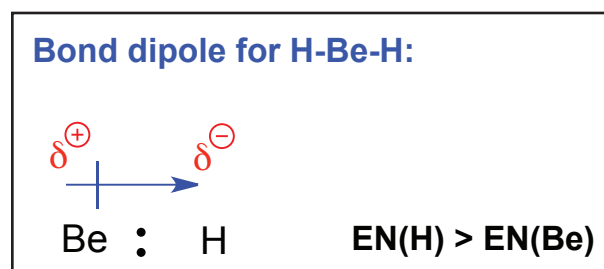
Ans: anion or anionic

**Q: Beryllium hydride is a covalent compound. Using the periodic table of electron configurations above, determine how many covalent bonds are to be expected for this metallic hydride?**

Ans: By sharing its two electrons or by forming a  $\text{Be}^{+2}$ , this Be atom either can get closer to or by ionization get to an He like electron configuration.

**Q: How does the difference in EN between Be and H affect the distribution of electrons in beryllium hydride? Draw the direction of a Be-H bond dipole.**

Ans: The EN of Be is 1.5 and the EN of H is 2.1. A Be-H bond is polar covalent with a  $\Delta\text{EN}$  of 0.6 with Be bearing a partial cationic charge and H a partial anionic charge.



**Q: How many covalent bonds can a carbon atom be expected to form?**

Ans: carbon has a **valence** electron configuration of  $2s^22p^2$ . Carbon needs 4 electrons to get to a Ne electron configuration. Carbon needs to form 4 bonds to get access to those 4 additional valence electrons.

**Q: If a carbon atom was to form an anionic species, what is the greatest amount of anionic charge that could most likely be accommodated by a carbon atom?**

Ans:  $2s^22p^2 + 4e^-$  will create a  $\text{C}^{-4}$  anion with a  $2s^22p^6$  electron configuration.

**Q: How many covalent bonds can a nitrogen atom be expected to form?**

Ans: Nitrogen has a  $2s^22p^3$  electron configuration, Nitrogen needs 3 electrons to get to a Ne like configuration. Nitrogen needs to form 3 covalent bonds to get access to those 3 additional valence electrons.

Whether or not a bond is ionic depends on the degree to which “shared” electrons are transferred from one atom to another atom. This degree of electron transfer not only depends on the difference of EN between two bonding atoms, BUT ALSO on whether the newly formed bond is between metallic and non-metallic atoms, or between two non-metallic atoms.

**Q: Is a CeF bond best described as an ionic or covalent? ionic**

Ans:  $\Delta\text{EN}(\text{Ce-F}) = 3.7$

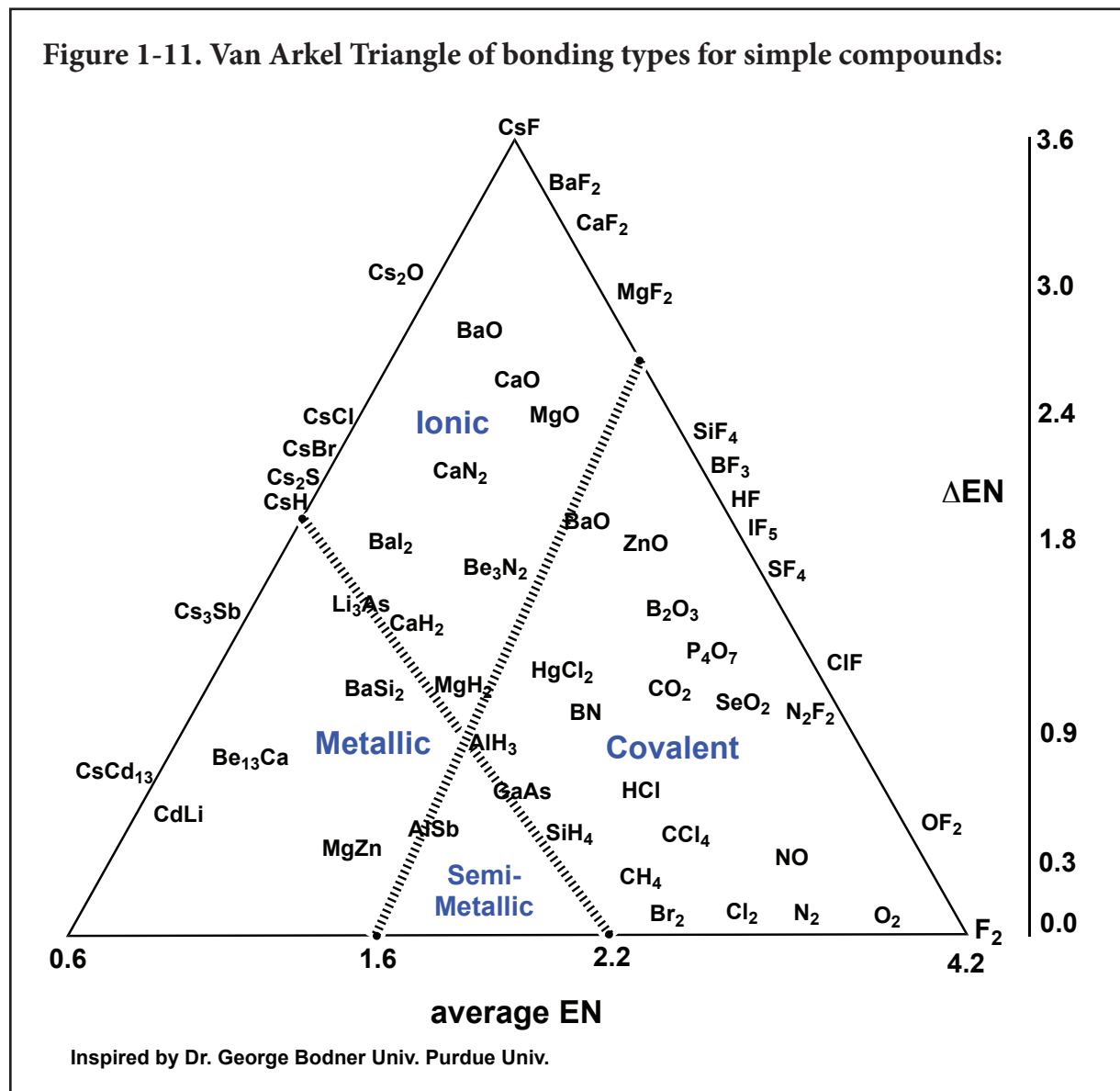
Ce is a metallic Element; F is a non-metallic element

**Q: Is  $\text{SF}_2$  formed from an ionic or covalent bonds? Polar covalent**

Ans:  $\Delta\text{EN}(\text{S-F}) = 1.5$

S is a non-metallic Element; F is a non-metallic element

A Van Arkel and Ketelaar triangle of bonding types for some simple binary combinations of elements demonstrates how both EN and the difference between EN ( $\Delta EN$ ) influence whether a bond between atoms is dominated by ionic, polar covalent or covalent types of bonds:



This Van Arkel bond triangle illustrates that these different types of bonding also are part of a continuum of interactions between atoms sharing valence electrons. Contrary to our expectations, based on bond type definitions, the data in the Van Arkel diagram illustrates that the differences between these various types of bonding are fuzzy at best. As Table 1-2 illustrates, even a bond that is described as ionic (e.g. Rb-F) still has a small contribution (i.e. ~8%) from a covalent bonding

interaction between  $\text{Rb}^{+1}$  and  $\text{F}^{-1}$  ions. Thus heterodiatom chemical bonds are not either covalent or ionic, but rather a combination of both bonding types. To say that an A-B bond is polar covalent is to say that the covalent bonding between A & B makes a larger contribution to the A-B bond than does an ionic bonding interaction between A & B.

**Table 1-2.  $\Delta\text{EN}$  and % of covalent character in polar covalent and ionic chemical bonds:**

$\Delta\text{EN}$	% Ionic	% Covalent
0.0 (e.g. X-X)	0.0	100
0.5	6	94
1.0 (e.g. ~HCl)	22	78
2.0	63	37
2.5	79	21
3.2 (e.g. Rb-F)	92	8

In Organic Chemistry, our focus will be on polar covalent bonds. Only a few special molecules can be described as *non-polar covalent*, i.e. those molecules containing purely covalent (100% covalent) bonds. Examples of homodiatom molecules include:



For such homonuclear diatomic molecules, the bonding electrons only can be evenly shared between these types of covalently bonded atoms. Just like other types of bonded atoms, homodiatom molecules either can be very stable (e.g.  $\text{N}_2$ ) or quite chemically reactive (e.g.  $\text{F}_2$ ,  $\text{H}_2$  and  $\text{Li}_2$ ).

Bonds between different atoms (e.g. A-B) are, by definition, polar covalent (i.e. that is < 100% covalent) because different atoms possess different values of electronegativity. These differences in electronegativity (e.g.  $\Delta\text{EN}$ ) between bonded atoms result in an unequal sharing of the bonding electrons (e.g. see Fig 1-10 above). This electron dislocation creates a partial transfer of electron density or a partial ionization of these shared or bonding electrons from the less electronegative atom to the more electronegative atom. As a result of this partial transfer of shared electrons, some additional partial ionic bonding or “ionic character” is added to what is essentially a covalent bonding interaction. A consequence of such ionic character is the creation of a dipole along this covalent bonding axis — a bond dipole (see Fig. 1-10):

## 1-6. Lewis Structures:

In addition to explaining some of the spectral features of atomic hydrogen, the Bohr model of the atom also accounted for the organization of Mendeleev’s Periodic Table. Bohr also noted that all of the Noble gases, except helium, contained an outermost shell of eight electrons. In 1916, G.N. Lewis formulated the *octet rule*, which postulated that an octet of electrons in the outermost shell of an atom was the most stable electron arrangement for an atom. This electronic stability is a force that drives atoms to form bonds to other atoms so that each of these bonded atoms can complete their individual octets. Gilbert N. Lewis, Nevil Sidgwick, and Herbert Powell used this idea to develop

a two-electron model for covalent bonding that explained many of the general valences observed for simple atomic combinations of the elements. This connection between the number of valence electrons around a central atom and the resulting geometry of that atom was developed into a more general application of this theory by Ronald Gillespie and Ronald S. Nyholm. They extended this Lewis theory into a formalism that generates 3-D Lewis structural representations, a theory now known as VSEPR theory (Valence Shell Electron Pair Repulsion Theory).

At the heart of determining a “best” Lewis structure for a covalently bonded molecule is the concept of formal charge. Formal charge (FC) is just a bookkeeping method for valence electrons. For the purpose of electron accounting, formal charge requires that all bonds between any two atoms be considered as if they are non-polar covalent- that is the bonding electrons are shared equally by any two bonded atoms (i.e. each bond is 100% covalent). Thus, any shared electrons are divided equally between these two bonded atoms. This value for formal charge is essentially a comparison of the valence electron distribution of a covalently bonded atom within a particular molecule to its corresponding valence electron count for a free and un-ionized atom:

**Figure 1-12: Formal charge definition and determination:**

### Formal Charge (FC):

**FC of X is FC(X) =**

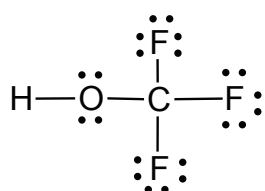
(free atom valence e<sup>-</sup> count for atomic element X) - [valence e<sup>-</sup> assigned to a bonded X]

**FC(X) =**

(old Group Numbering for an element X) - [ (Num. non-bonding e<sup>-</sup> on bonded X ) + 1/2(Num. e<sup>-</sup> covalently bonded to X) ]

As an example for how to calculate a formal charge, use the periodic table (top of each group column in Fig. 1-7 or 1-9), to determine the formal charge on C in the Lewis structure for HO-CF<sub>3</sub> below:

**Figure 1-14: Example Formal Charge calculation:**



Old Grp Num., Fig. 1.7

Num. of non-bonding elect.

Num. of bonding elect. to C

Using the formula above:  $FC(C) = 4 - [0 + 1/2(8)] = 4 - [0 + 4] = 4 - 4 = 0$

Thus, the formal charge on the carbon atom in this Lewis structure is  $FC(C)=0$

$FC(F) = 7 - [6 + 1/2(2)] = 7 - [6 + 1] = 7 - 7 = 0$

Thus, the formal charge on a fluorine atom in this Lewis structure is  $FC(F)=0$



**Q: Now you determine the formal charge on F for this HO-CF<sub>3</sub> Lewis structure?**

Ans:  $FC(F) = 7 - [6 + \frac{1}{2}(2)] = 7 - [6 + 1] = 7 - 7 = 0$

**Q: What is the formal charge on the O for this HO-CF<sub>3</sub> Lewis structure?**

Ans:  $FC(O) = 6 - [4 + \frac{1}{2}(4)] = 6 - [4 + 2] = 6 - 6 = 0$

**Q: How about FC for H this HO-CF<sub>3</sub> Lewis structure?**

Ans:  $FC(H) = 1 - [0 + \frac{1}{2}(2)] = 1 - [1] = 1 - 1 = 0$

Notice that if you add up the formal charges on all of the atoms in a molecule, you should get the overall charge on that molecule, if there is a charge.

**Figure 1-15: What is the overall charge on HO-CF<sub>3</sub>?**

Total Charge on HO-CF<sub>3</sub> =  $FC(H) + FC(O) + FC(C) + 3FC(F)$

Total Charge on HO-CF<sub>3</sub> =  $0 + 0 + 0 + 3(0) = 0$

### 1-7. Useful Algorithm for generating Lewis Structures (creator unknown):

One begins this process by using the molecular formula to make a tabulation of all available valence electrons;

#### Step 1: Determine number of valence electrons for molecular formula.

For each atom find its old Group Number (see Fig. 1-7 or 1-9). Do this for each atom in the molecular formula.

Then total up the number of these atomic valence electrons for all of the atoms in this molecule.

Finally look to see if this molecular unit has a total ionic charge. If this charge is negative, then **ADD those extra electrons** to your tabulated sum of valence electrons. If instead, this charge is **positive charge then SUBTRACT that number of electrons** from your total number of valence electrons.

#### Step 2: Determine the number of bonding electron pairs.

To determine the number of electron pairs available for covalent bonding within this molecule, divide your totaled number of valence electrons by 2.

#### Step 3: Generate preliminary Lewis structure.

In order to draw a Preliminary Lewis Structure:

First, select a central atom (typically it will be that atom with the **LOWEST** ionization potential or highest atomic number).

Place all of the other atoms around that selected central atom (a circular array is fine).

Connect those pendent atoms that surround the central atom to that central atom using one electron pair for each its remaining pendant atoms. Each pair of electrons used is subtracted from your total set of available electron pairs available for that molecular unit.

Next, use any remaining electron pairs to complete the octets on all the attached pendent atoms. Finally, any remaining electron pairs, and any odd extra electrons are placed onto the central atom.

From this preliminary Lewis structure one can predict both an electronic geometry (i.e. aka electron distribution or electron pair geometry), and then also a molecule's molecular shape. (See the Fig. 1-16 and 1-17)

#### **Step 4: Determine formal charges for atoms that form preliminary Lewis structure.**

In order to optimize the electronic geometry of a preliminary Lewis structure you'll need to determine the formal charges on all of the atoms within this preliminary Lewis structure.

Formal Charge(FC):

$$\text{FC}(X) = (\text{Group Num. for element X}) - [(\text{Num. non-bonding e- on bonded X}) + 1/2(\text{Num. e- bonded directly to X})]$$

After calculating formal charges a few times, you'll see that certain patterns of electrons on a particular atom will result in specific formal charges for that type of bonded atom. As you get more experience you won't need to calculate all the formal charges in a molecular unit to make a total FC count for a molecular unit. (e.g. see Table 1-3 below)

**\*\*Caution: Make sure that you take the time to calculate the formal charge for any central atom.**

To validate your determination of all formal charges: Simply sum of all formal charges that you have determined for all the atoms in that molecular unit. If your FC determinations are correct, then this sum will match the total ionic charge on that molecular unit.

#### **Step 5: Generate best Lewis structure.**

Optimize a preliminary Lewis structure by shifting those nonbonding electron pairs on the pendent atoms to make a new covalent bonding e- pairs to their central atom. The goal is to share enough pendent electrons to drive the formal charge of a central atom in a preliminary structure to zero or a negative number.

However, this sharing of pendant electron density has limits:

**Do not exceed an octet of electrons** if the central atom belongs to the **second row** of the periodic table.

**You can exceed** an octet for those central atoms that belong **to the 3rd or higher rows** of the periodic table.

In refining a preliminary Lewis Structure, your objective in sharing adjacent non-bonding electrons on a pendant atom with a central atom is to reduce the formal charge on that central atom. Forming

multiple bonds with pendant atoms reduces the Formal Charge on a central atom. You should form just enough double bonds with available pendant atom to drive a central atom's formal charge to zero or to a negative number.

### Checking final Lewis structures for errors:

1. **Atom check:** does your Lewis structure have the same number and atom types as the molecular formula?
2. **Does your structure have the correct number of valence electrons?**
3. **Octet Check:** Does each second row atom in your Lewis structure have a complete octet?
4. **Do the formal charges for your Lewis structure add up to the total or net charge on this molecular formula?**

Below in Table 1-3 is a quick guide to typical patterns of Formal Charges for bonded atoms frequently encountered in Organic Chemistry:

**Table 1-3. Shortcut guide to determination of Formal Charge:**

Grp Num.	Structures with +1 formal charge	Structures with 0 formal charge	Structures with -1 formal charge
3		—B— 	 —B <sup>⊖</sup> — 
4	—C <sup>⊕</sup> — =C <sup>⊕</sup>                ≡C <sup>⊕</sup>	—C— =C                ≡C—	—C <sup>⊖</sup> — =C <sup>⊖</sup>                ≡C: <sup>⊖</sup>
5	—N <sup>⊕</sup> — =N <sup>⊕</sup>                ≡N <sup>⊕</sup>	—N— =N—                ≡N:	—N <sup>⊖</sup> — =N <sup>⊖</sup> 
6	—O <sup>⊕</sup> — =O: <sup>⊕</sup> 	—O— =O: 	—O: <sup>⊖</sup>
7	—X <sup>⊕</sup> : X = (F, Cl, Br, I)	—X: : :	: X: <sup>⊖</sup> :

In Table 1-3, each line represents a 2e<sup>-</sup> covalent bond, dots represent non-bonding e<sup>-</sup> pairs, the charges + and - refer to formal charges of (+1) and (-1) respectively on that central atom for that type of bonding environment (i.e. electronic geometry).

### Q: For BH<sub>3</sub>; what is the formal charge on B?

Ans : 0 (Look for B with 3-bonds, then look at column heading in Table 1-3)

Using formula  $FC(B) = 3 - 1/2[0 - 1/2(6)] = 3 - 3 = 0$

## 1-8. Oxidation Number (Ox):

At the other end of this valence electron bookkeeping spectrum is the concept of *oxidation number* or *oxidation state*. Oxidation Number also is a bookkeeping technique for valence electrons. The calculation of oxidation number is similar to that done for formal charge except for one very important assumption: For an oxidation number, all bonds between any two atoms are considered as ionic — that is all of the bonding or shared electrons belong to the most electronegative atom in a bonded pair of atoms.

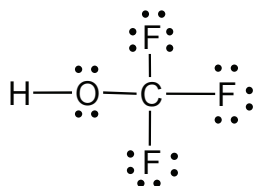
### Eq. 1-3:

$$\text{Ox of X is } \text{Ox}(X) = (\text{valence } e^- \text{ count for element X}) - [\text{valence } e^- \text{ assigned to X}]$$

$$\text{Ox}(X) = (\text{Group Num. for element X}) - [(\text{Num. non-bonding } e^- \text{ on bonded X}) + (\text{Num. } e^- \text{ bonded to that are assigned to X})]$$

By the definitions above, the oxidation number of an element (e.g. Na or Na<sub>2</sub> or O<sub>2</sub>, etc.) is 0.

Let's calculate an oxidation number for C in HO-CF<sub>3</sub>.



$$\text{Ox}(C) = 4 - [0 + 0] = 4 - [0] = 4$$

$$\text{Ox}(C) = +4$$

Since oxidation number is not sensitive to the number of shared electrons, it too can be determined from a preliminary Lewis structure, along with molecular shape, and an electronic geometry.

**Q: Determine Lewis Structure for CH<sub>4</sub> and also FC(C) and OX(C):**

$$\text{Ans: FC}(C) = 4 - [4] = 0$$

$$\text{Ox}(C) = 4 - [0 + 8] = -4$$

**Q: Determine FC(C), FC(H) and also OX(C) for an ethylene or ethene molecule: H<sub>2</sub>C=CH<sub>2</sub>**

$$\text{Ans: FC}(C) = 4 - [0 + 4] = 0$$

$$\text{Ox}(C) = 4 - [0 + 6] = -2$$

$$\text{Ox}(H) = 1 - [0 + 0] = 1$$

**Q: Determine FC(C) and also OX(C) for a formaldehyde molecule: H<sub>2</sub>C=O**

$$\text{Ans: FC}(C) = 4 - [0 + 4] = 0$$

$$\text{Ox}(C) = 4 - [0 + 4] = 0$$

**Q: Determine FC(C) and also OX(C) for an acetylene molecule: H-C≡CH**

**Ans: FC(C)=4-[0+4]=0**

**Ox(C)= 4 - [0+5]= -1**

**Q: Why should an Atom's FC change as one alters its covalent bonding, but not an atom's oxidation number?**

**Ans: For oxidation number, shared electrons are assigned to a particular atom; that assignment does not depend on the number of electrons shared between atoms. This is not true for formal charge.**

The concept of Formal Charge is a bit more important than oxidation number for two reasons:

1. FC is used to determine an optimal valence electron distribution for a given Lewis structure
2. Formal charge often is transferred from one atom to another during a chemical reaction and those transferred electrons must be conserved during a reaction. The use of formal charge is an important tool used to track electron transfers in order to develop reaction mechanisms.

**Eq. 1-4: Example: protonation and proton transfer reactions:**



In the reaction described by Eq. 1-4, formal charge is conserved: That is, the +1 charge on the proton is transferred to the oxygen atom in its reaction with water to produce  $\text{H}_3\text{O}^+$ .

Here are some sample problems to consider before leaving this chapter:

**Q: Draw a Lewis structure for  $\text{NF}_3$**

Ans:

Step1.  $1\text{N} = 1 \times 5 = 5$ ;  $3\text{F} = 3 \times 7 = 21$ ; total  $e^- = 5 + 21 = 26e^-$  or

Step2: 13  $e^-$  pairs

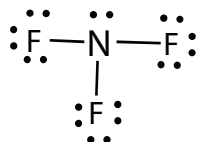
Step3a: Central atom is N, lowest ionization energy .

Step 3b: N surrounded by 3 F atoms

Step 3c: use 3 pairs of  $e^-$  to bind each F to the N-atom

Step 3d: use 9 pairs of  $e^-$  to complete the octets of all F atoms.

At this point, we have used 12  $e^-$  pairs so add the last  $e^-$  pair to the central N atom.



Now calculate  $\text{FC}(\text{N})$  , see next Q

**Q: What is the  $\text{FC}(\text{N})$  for the preliminary structure above? For the final or best Lewis structure?**

Ans:  $\text{FC}(\text{N}) = 5 - [2 + 1/2(6)] = 5 - 5 = 0$ , In the preliminary structure N has a complete octet, and because N is a second row element, it cannot expand beyond its octet. Thus the preliminary Lewis structure for  $\text{NF}_3$  is also the best Lewis structure for  $\text{NF}_3$

**Q: What is  $\text{Ox}(\text{F})$ ?**

Ans:  $\text{EN}(\text{F}) > \text{EN}(\text{N})$ , thus  $\text{Ox}(\text{F}) = 7 - [6 - 2] = -1$  ,  $\text{Ox}(\text{N}) = 5 - [2 + 0] = +3$

**Q: Draw a Lewis structure for  $[\text{SO}_3]^{-2}$**

Ans:

1.  $1\text{S} = 1 \times 6 = 6$ ;  $3\text{O} = 3 \times 6 = 18$ ,  $-2\text{charge} = +2$ ; total  $e^- = 6 + 18 + 2 = 26 e^-$  or

2. 13  $e^-$  pairs

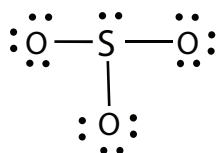
3a. central atom is S

3b. S surrounded by 3 O atoms

Step 3c: use 3 pairs of  $e^-$  to bind each O to the S-atom

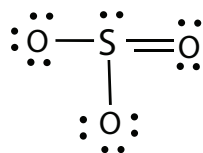
Step 3d: use 9 pairs of  $e^-$  to complete the octets of all O atoms.

At this point, we have used 12  $e^-$  pairs so add the last  $e^-$  pair to the central S atom. This preliminary Lewis structure also is like that of  $\text{NF}_3$ .



**Q: What is the FC(S) for the preliminary structure? For the final or best Lewis structure?**

Ans:  $FC(S) = 6 - [2 + \frac{1}{2}(6)] = 6 - [2 + 3] = 6 - 5 = +1$ . Sulfur is an element in the 3rd row, and can expand its octet. If one of the oxygen atoms shares a non-bonding pair of electrons with S, the FC(S) for this final structure will be 0:



Ans: Best Lewis structure for  $[SO_3]^{-2}$

**Q: What is Ox(S) for BOTH the preliminary Lewis and final or best Lewis structures of  $[SO_3]^{-2}$ ?**

For both structures:  $EN(O) > EN(S)$ , thus  $Ox(S) = 6 - [2 + 0] = 6 - 2 = +4$

## 1-9. Electronic geometry (i.e. electron distribution) and its relation to molecular shape:

You will have noticed that a Lewis structure consists of a central atom (i.e. A), and its pendant atoms (i.e. X) bonded to that central atom. In addition that central atom sometimes also may contain a number of non-bonding electron pairs (i.e. E). Thus any Lewis structure can be reduced to an  $AX_mE_n$  notational representation. For  $NF_3$ , this molecule now becomes an example of an  $AX_3E$  type of Lewis structure.

Now that one has a “best” Lewis structure for a molecule, just what does it look like in 3-dimensions? This turns out to be a slightly complicated question. Molecular structures are described by two important terms: *Electronic Geometry*, and *Molecular Shape*. Although related, they are not interchangeable.

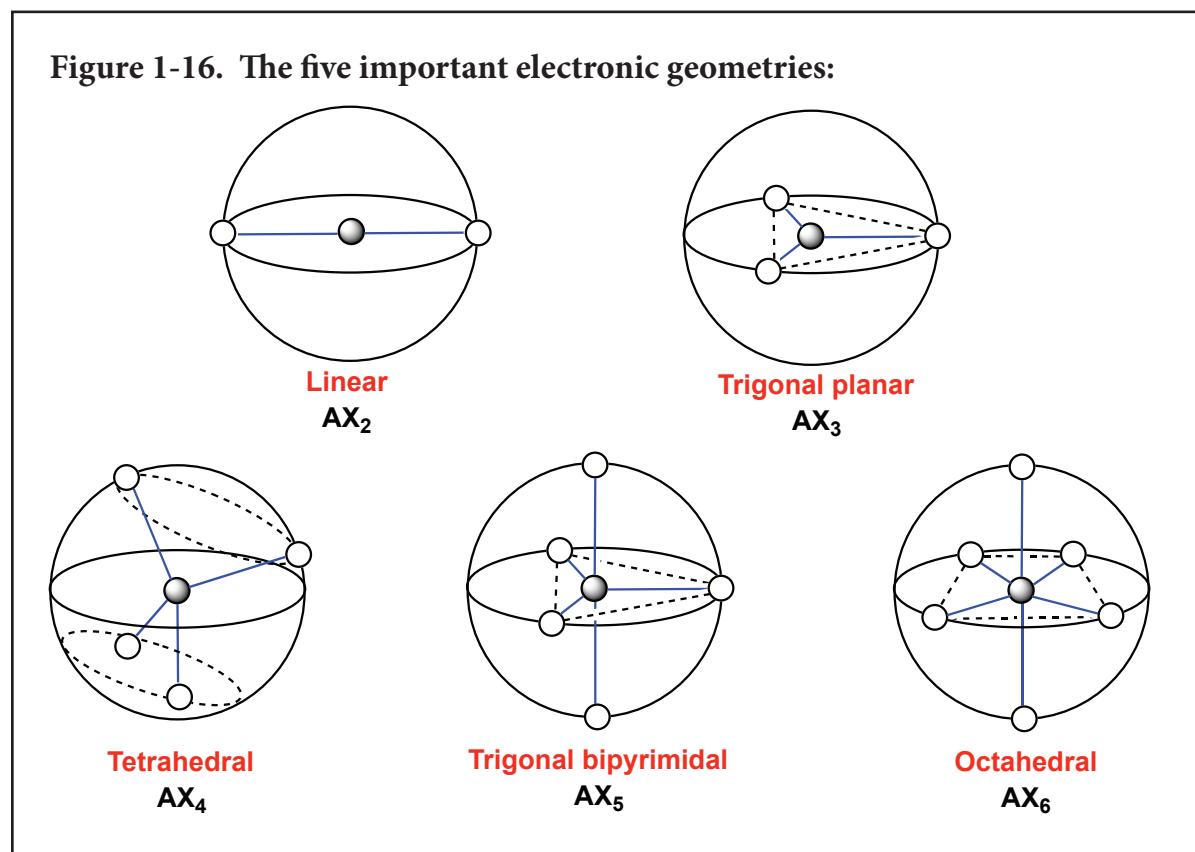
Electronic geometry depends on the number of both bonded atoms and also non-bonding electron pair orbitals attached to a central atom. Those orbitals filled with non-bonding electrons and those shared electron pairs in their covalent bonds, will orient themselves in space so that all of these valence electron pairs can be as far apart from each other in space as is possible (i.e. recall Coulomb’s Law-that like charges repel like charges). In the VSEPR (valence shell electron repulsion) theory, this repulsion among these various electron pairs generates an electronic geometry for that central atom.

Molecular shapes are determined by counting **only** the number of bonded atoms attached to a central atom. This makes sense because usually it’s experientially easier to “see” atomic positions. Electron positions have to be inferred using more indirect methods. Thus a molecular shape depicts only the number of atoms bonded to a central atom. These two structural properties (i.e. electronic geometry and molecular shape) are related as children are to their parents-electronic geometry is the parent to a molecular shape.

The theory that is most often used to sort out these related structural properties of Lewis structures is called VSEPR (valence shell electron pair repulsion). This model assigns 3-D electron arrangements around a central atom in a Lewis structure based on the simple idea is that the valence electrons

around a central atom repel each other. Thus all covalent bonds and any non-bonding pairs of electron orbitals bonded to a central atom adopt geometries that minimize these electron repulsions around their central atoms. Maximum electron pair separation around a central atom is achieved by arraying all of the occupied bonds and orbitals so that they are splayed out as far apart in space as is possible from each other.

Like Platonic solids, there are five common electronic geometries, or what technically also are referred to as electron distribution geometries about a central atom:

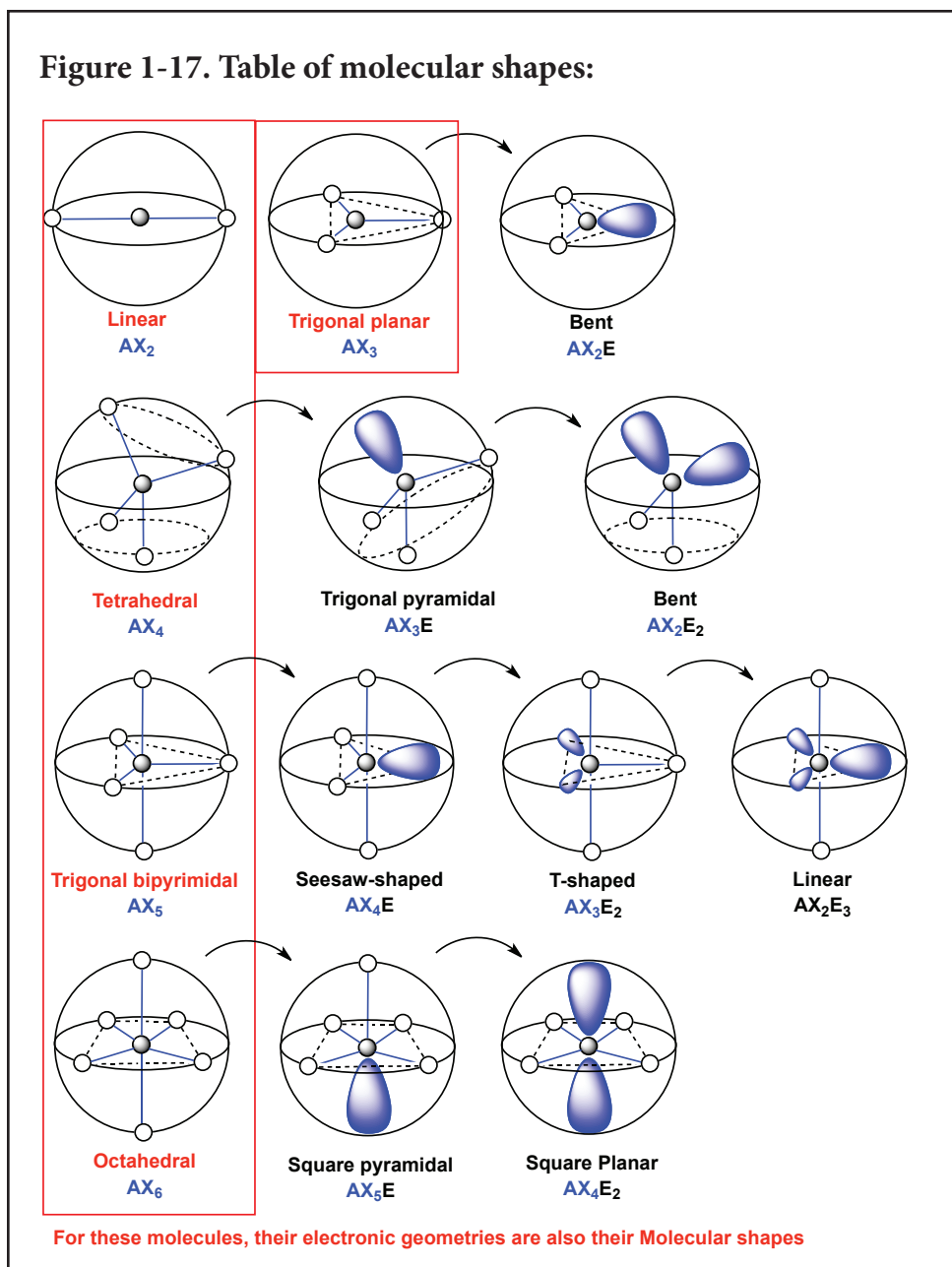


Each of one these five different electronic geometries can give rise to a variety of possible molecular shapes that also will have the same electronic geometry. In some cases, the electronic geometry and molecular shape are identical. A good example of this is methane ( $CH_4$ ). Methane has both a tetrahedral electronic geometry AND a tetrahedral molecular shape.

However, molecular shapes are organized only around the number of atoms bound to a central atom. As a result, depending on the number of bonded atoms, each of the electronic geometries can give rise to a variety of molecular shapes. Thus our  $AX_3E$  Lewis electronic structure belongs to the  $AX_4$  family of Lewis structures:  $AX_4$ ,  $AX_3E$ ,  $AX_2E_2$ ,  $AXE_3$  all of which have tetrahedral electronic geometries, but each structure with similar electron distributions or geometries has a different molecular shape (Figure 1-17 below). Typically, the more atoms and non-bonding electrons around a central atom, the greater the number of possible molecular shapes:



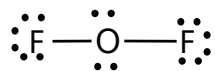
Figure 1-17. Table of molecular shapes:



The  $AX_3E$  Lewis structure of  $NF_3$  belongs to the  $AX_4$  family of Lewis electron geometries. Although the molecule  $NF_3$  has a tetrahedral electronic geometry, one notes from Figure 1-17 above that  $AX_3E$  has a trigonal pyramidal molecular shape. The importance of this distinction is that molecules of different shapes often share similar electronic geometries; and these electronic geometries generally are more important to chemical reactions than molecular shapes. For example, consider the molecules:  $CH_4$ ,  $NH_3$ ,  $H_2O$  and  $H-F$ . They all have different molecular shapes, but they also all have central atoms that possess tetrahedral electronic geometries. As you can see from Figure 1-17, there are a number of molecular shapes that can be derived from different electronic geometries, and this is why it is important to establish electronic geometry prior to determining a molecular shape.

There is one final observation worth noting that often can save the reader some effort if ONLY an electronic geometry and molecular shape are desired for a simple molecule. One doesn't have to use a "best" Lewis structure to make this determination. One can assign electronic geometry and molecular shape using only a preliminary Lewis structure generated by the algorithm in Section 1-7. Remember, ignoring this algorithm, can lead one to generate incorrect preliminary Lewis structures. These incorrect structures, in turn lead to erroneous assignments of electronic geometries and their associated molecular shapes.

**Q: The Lewis structure for  $\text{OF}_2$  is:**

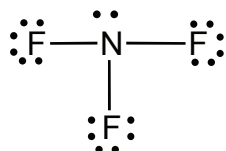


**This molecule has:**

**an electronic geometry that is?** [Ans: tetrahedral](#)

**and a molecular shape that is?** [Ans: bent](#)

**Q: The Lewis structure for trifluoroamine is:**

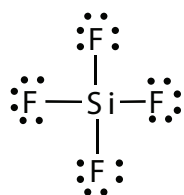


**This molecule has:**

**an electronic geometry that is?** [Ans: tetrahedral](#)

**and a molecular shape that is?** [Ans: trigonal pyramidal](#)

**Q: The Lewis structure for tetrafluorosilane ( $\text{SiF}_4$ ) is:**



**This molecule has :**

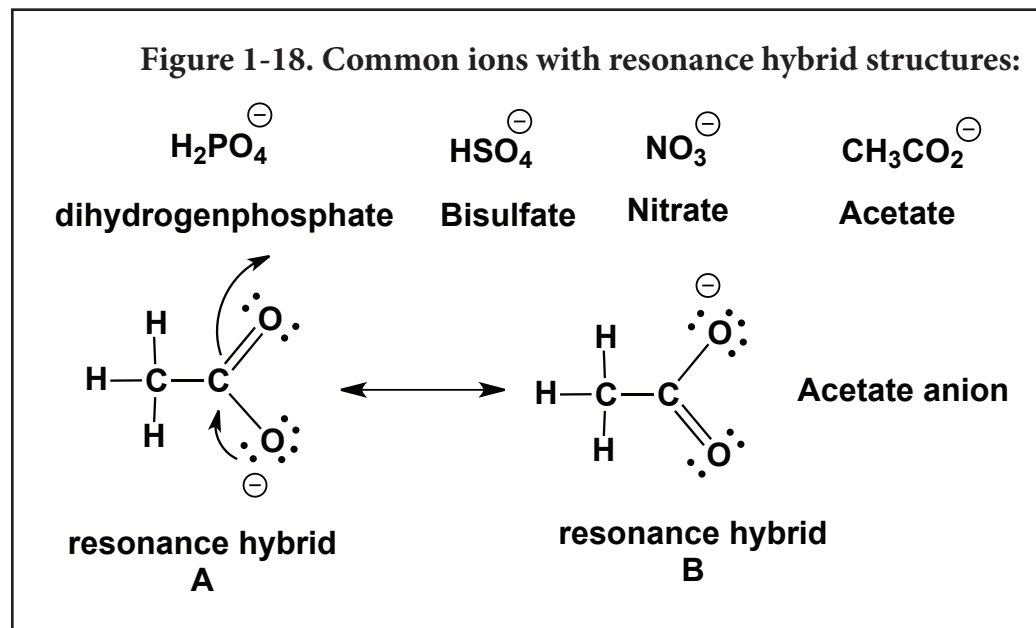
**an electronic geometry that is?** [Ans: tetrahedral](#)

**and a molecular shape that is?** [Ans: tetrahedral](#)

Notice that  $\text{OF}_2$ ,  $\text{NF}_3$  and  $\text{SiF}_4$  all have the same type of electronic geometry, however, they each have different molecular shapes because each has a different number of bonded atoms around their central atom.

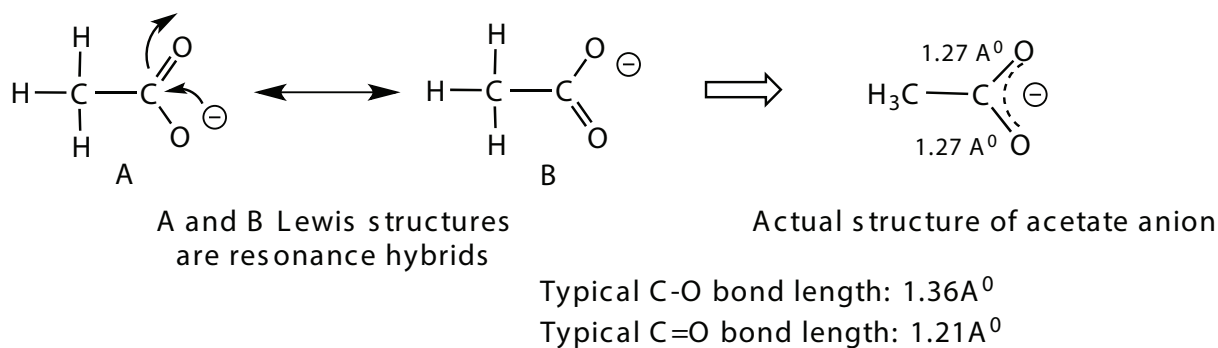
## 1-10. Resonance:

Resonance is a concept necessary for certain Lewis structural representations. Resonance is not a quantum mechanical concept-conjugation or delocalization is a quantum mechanical concept. The reader has or should have been exposed to the resonance concept in those Lewis representations for several common inorganic anions:



The Lewis definition of resonance generally is associated with equivalent multiple Lewis representations for a particular molecular structure. Resonance is used for those structures that have electrons shared between more than two adjacent atoms within that structure. Resonance hybrid structures are imaginary — that is they do not have an independent existence — resonance is **NOT** a special type of fast equilibration process. Instead, the actual or “real” structure is an energy weighted average or “mixture” of its resonance hybrid structures. For example, when one determines the X-ray structure for an acetate ion, one does not observe two different C-O bond lengths (i.e. a long one for one for a C-O bond and another, shorter one, for a C=O bond). Instead one observes two C-O bonds with the same length. These C-O bond lengths also are intermediate in their lengths somewhere between a typical value for C-O single bond length and a value typical for C=O bond length (Fig. 1-19):

**Figure 1-19. How resonance hybrid structures affect actual bond lengths:**

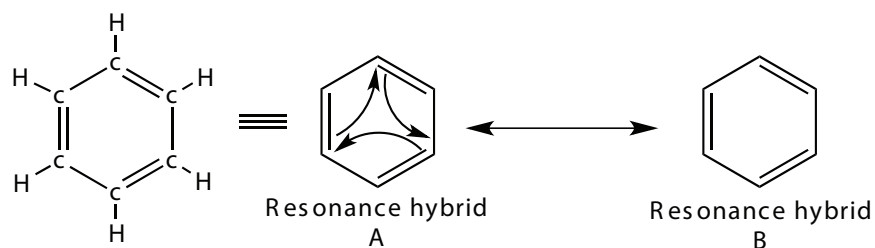


The reader also might recall from General Chemistry, that the general guidelines for resonance structures are:

1. Resonance hybrids involve shifts in electrons — NOT shifts in atomic positions.
2. For elements belonging the first and second row, completed octets are more important (i.e. such resonance hybrids are lower in energy—more stable than structures with unfilled octets).
3. For resonance hybrids that involve charge separation, those resonance hybrids that place additional electron density on the more electronegative atoms contribute more to an actual structure of a molecule. These types of ionic resonance hybrids are more stable — lower in energy — than those ionic resonance hybrids that place positive charge onto a more electronegative atom.
4. The more important ionic structures (more stable — lower in energy) also will minimize the separation distance between different ionic charges.

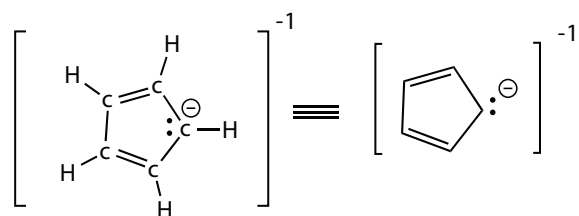
Resonance by itself is a necessary but not a sufficient condition for conjugation (resonance is only a concept of Lewis structures). Resonance just indicates that conjugation is possible, but resonance does not reveal anything about the strength of that conjugation.

e.g. Benzene—is one of the most conjugated molecules known to date:

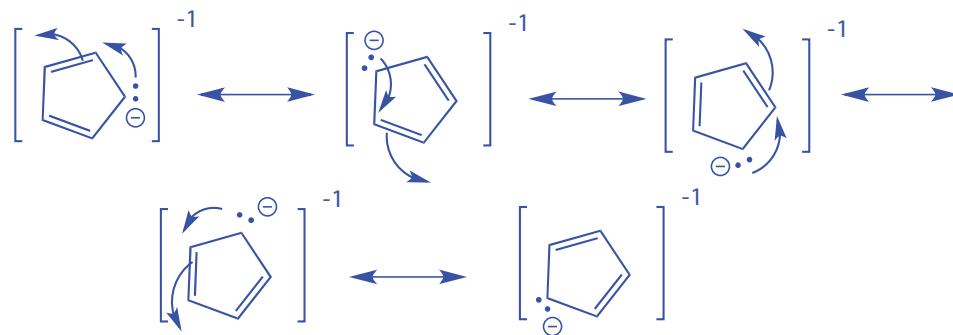


*For future Reference: Just because one can draw resonance hybrids for a given Lewis structure does not mean that a molecular structure is conjugated, nor does it reveal how much that conjugation contributes to a given molecular structure. This qualification will make more sense when we discuss conjugation again in Chapter 16.*

**Q: Draw all simple resonance hybrid contributions for the cyclopentadienyl anion below:**



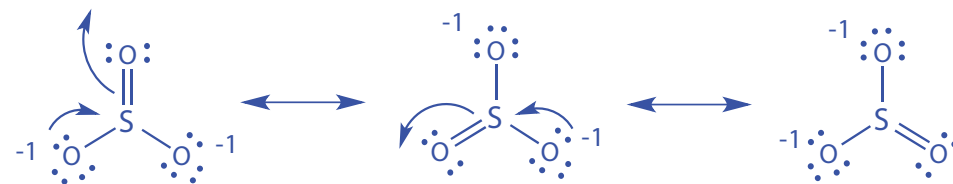
Ans:



**Q: For  $[\text{SO}_3]^{-2}$  ion, how many identical resonance hybrid structures are possible?**

**Draw them?**

Ans:

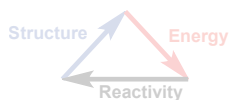


## 1-11. Conclusion:

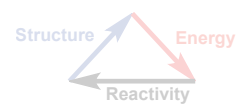
For some readers a bit of time may have passed since they took General Chemistry and considered chemical bonding. Chemical bonding affects the essential properties of molecules, including their structural stability, chemical reactivity, and physical properties. Lewis structures provide an access into the three dimensional nature of covalently bonded molecular structures that are based on component atomic electronic structures. In addition, Lewis structures are important because they form a foundation for all structural representations used in chemistry and particularly in Organic Chemistry. In subsequent chapters we will build upon this theoretical knowledge of atomic electronic structure to describe both the structure and reactivity of organic molecules.

## 1-12. What you should know and be able to do:

1. Identify the elements and their symbols for the Blue atoms in the main groups of the Periodic Table.
2. Locate and name the parts of an atom important to chemistry.
3. Interpret the information provided by a chemical symbol.
4. Name and identify the orbital properties described by the quantum numbers.
5. What sets of quantum numbers mean and what values are possible for a given value of  $n$ , including the different atomic orbitals: s,p,d
6. Write out a ground state electron configuration for any first or second row element.
7. Describe the relationship between electron configurations and the organization of the Periodic Table.
8. Explain periodic table trends, such as, how does ionization energy increase as one moves from left to right along a row in the periodic table?
9. Why do atoms react to form chemical bonds?
10. What are the types of chemical bonds that are important to Organic Chemistry?
11. What is electronegativity and what are the trends in EN as one moves across a row or down a column in the Periodic Table?
12. Describe the bonding within a homodiatomic molecule.
13. What determines the magnitude and direction of a bond dipole?
14. Construct both a preliminary and best or final Lewis structure from a molecular formula.
15. Determine the formal charge (FC) for atoms within a Lewis Structure.

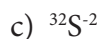


16. Determine the electronic geometry and molecular shape of a Lewis structure.
17. Determine the oxidation number (Ox) for atoms within a Lewis structure.
18. Identify and draw proper resonance structures.



### 1-13. Problems:

1. How many Protons, neutrons, and electrons in the following atoms: ans(P,N,e)



2. For an atom of the element  $^9\text{Be}$ , describe the number, type of its various subatomic components important to chemistry, and where they are located in an atom of Be.

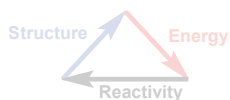
3. Why does the atomic mass of an element seem to ignore the mass of its electrons?

4. Write ground state electron configurations for the atoms below:



5. How many electrons can have quantum number designations:  
 $n=3, l=0$  and  $S$  or  $M_s = \frac{1}{2}$  and what types of orbitals can they occupy?

6. Which of the species listed below can have the electron configuration  $3s^2 3p^6$  as their highest principle quantum energy level?  $\text{Ca}^{+2}$ ,  $\text{Na}^{+1}$ ,  $\text{Ne}$ ,  $\text{Ar}$ ,  $\text{F}^{-1}$ ,  $\text{Cl}^{-1}$





7. Which of the following ions possesses the electron configuration of a noble gas (isoelectronic with a noble gas). Also specifically identify which noble gas?

- a)  $\text{Li}^{+2}$
- b)  $\text{Cl}^{+1}$
- c)  $\text{O}^{-2}$
- d)  $\text{H}^{-1}$
- e)  $\text{Mg}^{+1}$

8. What is the ordering of radii for the following atoms? Use the proper symbol for each element and organize the sequence from the smallest radii on the left to the largest radii on the right:

a) fluorine, carbon, neon, oxygen, nitrogen

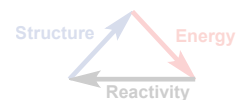
b) What are two atomic properties that correlate with your smallest to largest radii sequence above?

9. If one makes ions of the following elements, then what will be the ionic charge that would produce an ion that is isoelectronic with its **nearest** noble gas electron configuration?

- a) B
- b) P
- c) Cl
- d) Mg
- e) Be

10. Based on electron configurations, what is the expected molecular formula for the following proposed compounds

- a) Lithium and chlorine
- b) Tin and oxygen
- c) Boron and nitrogen
- d) Oxygen and fluorine
- e) Strontium and nitrogen



11. Draw an atomic orbital diagram for the ground state electron configuration of nitrogen; most stable orbital energy at the bottom, least stable orbital energy at top of diagram:

- What is the principle quantum number for nitrogen's valence electrons?
- What are the highest energy orbitals?
- What molecular formula would you predict for a molecule composed of nitrogen and iodine?

12. Which is the more electronegative atom in each bonded pair of atoms?

- C-N
- O-N
- C-H
- Cl-Br
- B-C
- Li-C
- C-F
- Si-F
- H-F

13. Identify the following bonds as ionic, polar covalent, or covalent:

- Na-F
- H-Br
- Cl-I
- H<sub>2</sub>N-H
- Na-OCH<sub>3</sub>

14. What are the directions for the bond dipoles for the bonds as they are drawn below?

a) C-N

b) O-N

c) C-H

d) Cl-Br

e) B-C

f) Li-C

15. Rank the following bonds in order of increasing ionic character on the/a carbon atom:

(Ans: lowest to highest ionic character)

a)  $\text{H}_3\text{C}-\text{CH}_3$  b)  $\text{H}_3\text{C}-\text{MgBr}$  c)  $\text{H}_3\text{C}-\text{Li}$  d)  $\text{H}_3\text{C}-\text{F}$  e)  $\text{H}_3\text{C}-\text{OH}$  f)  $\text{H}_3\text{C}-\text{NH}_2$

16. Consider the following compounds and decide if they are likely to be ionic or non-polar covalent or polar covalent, and the basis for your decision:

a)  $\text{NF}_3$

b)  $\text{Na}_2\text{O}$

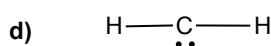
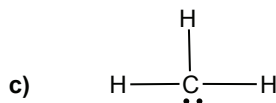
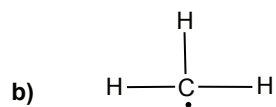
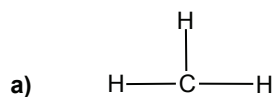
c)  $\text{CO}_2$

d)  $\text{Cl}_2$

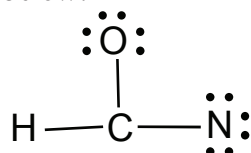
e)  $\text{CH}_4$

f)  $\text{LiF}$

17. What is the formal charge on the carbon atoms for the Lewis structures shown below?



18. What are the formal charges for O, C, and N on the preliminary Lewis structure for molecule below?



a) What are the oxidation numbers for C, O, and N for the Lewis structure above?

b) Draw the Best Lewis structure for the molecule shown above in Q17?

c) What are the formal charges for O, C, and N atoms in this Best Lewis structure?

d) What are the oxidation numbers for C, O, and N atoms in this best Lewis structure?

e) Did oxidation number depend on a Lewis structure (preliminary vs best)? How about formal charge?

f) Did the molecular shape of  $[\text{HCNO}]^{-2}$  change as a function of electron geometry for its different Lewis structures?

g) Did the electronic geometry around the central atom (i.e. C) change as a function of the changes in electron distribution in these Lewis structures?

19. Use arrow formalism to write possible resonance structures for the molecules below: (be sure to locate any changes to formal charge)

