Chapter 1

Review of General Chemistry

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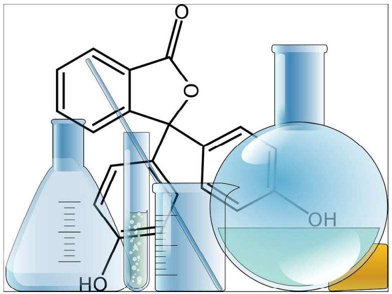

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1.1 Atoms and Molecules

From a chemistry prospective, all matter that exists is composed of a basic building block the **atom**. The origin of the term atom is the Greek word "atoms" which means indivisible and it was initially thought that atoms could not be divided into more fundamental parts of matter. This is untrue as each individual atom is composed of protons, neutrons and electrons and if one explores further each of those is further composed of other subatomic particles, though that deviates from a study of chemistry to that of physics.

There are a limited number of different types of atoms which we call elements (currently 118 elements have been discovered). Elements can combine together to form an almost unlimited number of compounds/molecules. If we think of atoms as the letters of the alphabet then compounds/molecules are the words formed from them. Just as the limited number of letters in the alphabet can be combined together to form words, sentences and eventually Shakespeare, so to can the elements be combined together to form compounds and molecules which gradually get larger and more complex until they eventually form a living human being.

Three Fundamental Particles

Protons have a relative mass of 1 amu, a positive charge and reside in the nucleus of the atom. The identity of each element on the periodic table is determined by the unique number of protons each has. Hydrogen has one proton, Helium has two and so on.

Neutrons have a relative mass of 1 amu, a neutral charge and also reside in the nucleus of the atom. They are important for the stability of the nucleus and elements which contain different numbers of neutrons are called isotopes. Isotopes are frequently used in many chemical techniques to determine the structure of molecules but have little impact on the physical and chemical properties studied in this book.

Electrons have a relative mass of 1/1832 amu, a negative charge and reside outside the nucleus of the atom. From the perspective of a chemist, electrons are the most important fundamental particle. Electrons

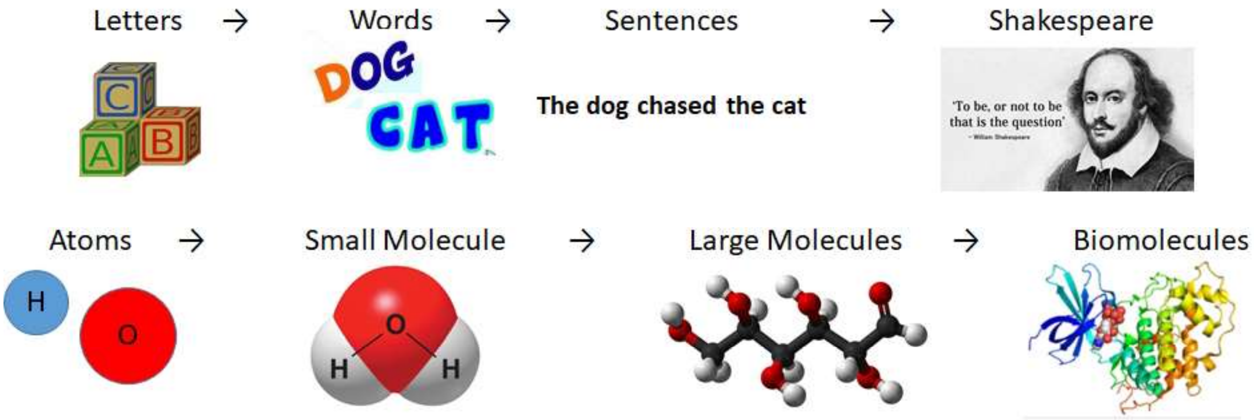


Figure 1.1 An analogy - chemistry (elements) and your english class (letters) are very similar. credit: author

are gained or lost to form ions which react to form ionic compounds. They are shared to form molecular compounds which includes most organic molecules studied in this book. Electrons essentially determine the chemistry we study.

Particle	Symbol	Charge	Mass	Location	Importance
Proton	p	+	1 amu	Nucleus	determines the element
Neutron	n	0	1 amu	Nucleus	determine the isotope
Electrons	e^-	-1	1/1832 amu	Cloud	determines chemical bonding and reactions

Table 1.1 Important properties of protons, neutrons and electrons

Cations and Anions

A driving force in the discovery of electrons (and protons) was the observation that some substances when dissolved in water conduct electricity and is attracted to the cathode (+) or anode (-) terminals of a battery. Atoms can gain or lose electrons to form charged ions. If an atom loses an electron the resulting ion is positive and called a cation. If an atom gains an electron the resulting ion is negative and called an anion. Multiple electrons can be lost or gained this way.

$$\begin{array}{rcl} \text{Cation are positive} & \text{(lose electrons)} & \mathrm{Na} \longrightarrow \mathrm{Na}^{+1} + e^- \\ \text{Anion are negative} & \text{(gain electrons)} & \mathrm{Cl} + e^- \longrightarrow \mathrm{Cl}^{-1} \end{array}$$

Chemists represent the charge on an ion using a trailing superscript to denote the number of electrons missing (given a positive sign to indicate the charge on the ion formed), or the number of electrons gained (given a negative sign to indicate the charge on the ion formed). Cations and Anions are important in organic and biochemistry due to the attractive and repulsive forces between the charges as discussed in the next section.

Coulomb's Law Many concepts in chemistry depend on the attractive and repulsive forces between charged (+ and -) or partially charged (δ^+ and δ^-) ions and molecules. The proprieties of charges can be summarized as follows:

1. Two types of charges: positive (+) and negative (-)
2. Opposite charges attract (+/-) and like charges repel (++ or - -)
3. Charges can be transferred. In chemistry this is achieved by gaining or losing electrons.

4. The attractive or repulsive force is directly proportional to the magnitude of the charges and inversely proportional to the distance between them.

$$F = k\frac{q_1 q_2}{r^2}$$

F - force of attraction or repulsion
q_1, q_2 - magnitude of charges
r - distance between charges
k - Coulomb Constant

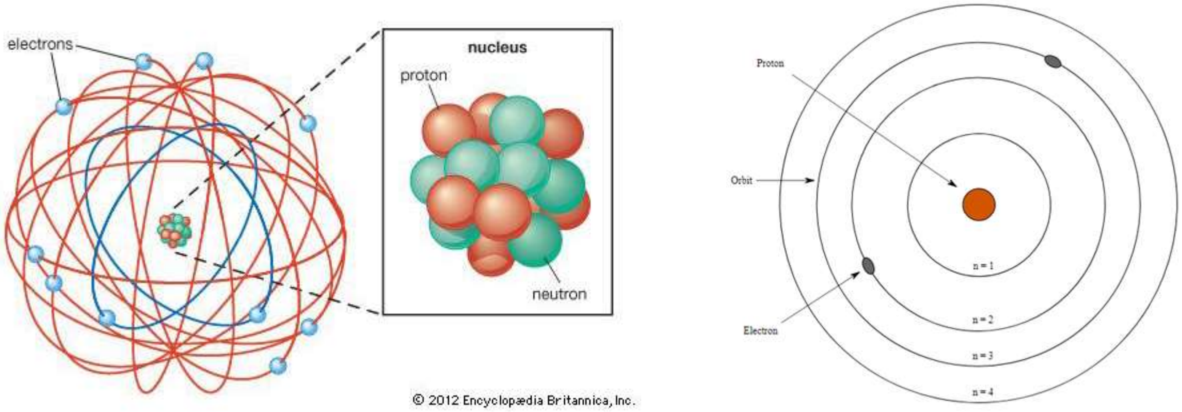
Figure 1.2 Coulomb's Law - describe the attractive or repulsive force between two charged particles. The force is directly proportional to the magnitude of the charges and inversely proportional to the distance between the charges

Coulomb's Law states that the force (F) associated with attraction or repulsion is directly proportional to the magnitude of the charges (q_1 and q_2) and inversely proportional to the distance (r) between the forces. In chemistry Coulomb's law is used to describe the interaction between protons and electrons in an atom, to describe the ionic bond formed between cations and anions (for example in Na^+Cl^-), to understand the sharing of electrons in covalent/molecular compounds, the solubility of compounds in water (and other solvents) and the Intermolecular Forces (IMF's) between molecules that explain many physical properties of compounds.

Models of the Atom

Understanding the structure of an atom, primarily the arrangement of electrons, is key to understanding the rules governing the formation of chemical bonds between atoms to form molecules. Over the course of time many models of the atom have been proposed, several of which will be explored here as each elucidates an important concept.

The **Rutherford Model** of the atom proposed that the protons and neutrons are located in a small, dense, and positively charged nucleus surrounded by a large cloud of negatively charged electrons. The attractive force between the electrons around the nucleus creates a stable atom and the attractive force between electrons to two different atoms nucleus results in the formation of a chemical bond.



(a)

(b)

Figure 1.3 (a) Rutherford Model of the Atom (b) Bohr Model of the Atom credit: a: `https://commons.wikimedia.org/wiki/File:22476-004-9B6970F9.jpg` b: `https://commons.wikimedia.org/wiki/File:Bohr's_model.svg`

Bohr Model The next major advance in the understanding of the atom was the Bohr model which placed the electrons in quantized orbitals. The electrons can be pictured like planets orbiting the sun with only certain distances between orbitals allowed. Only the electrons in the outer orbitals are allowed to be lost or gained to form ions and shared to form molecules.

De Broglie Model Electrons are very small, and don't follow the rules of classical mechanics which describes them as particles which orbit the nucleus. Instead we need to think of them as particles and waves (wave/particle duality). Waves can exhibit constructive (waves reinforce) and destructive (waves cancel) interference, this results in forbidden orbitals where destructive interference occurs and allowed orbitals where constructive interference occurs, explaining the quantization of orbitals. This duality also means that a planetary/orbital model is too simple to explain how electrons interact, leading to the development of the Quantum Mechanical model of the atom.

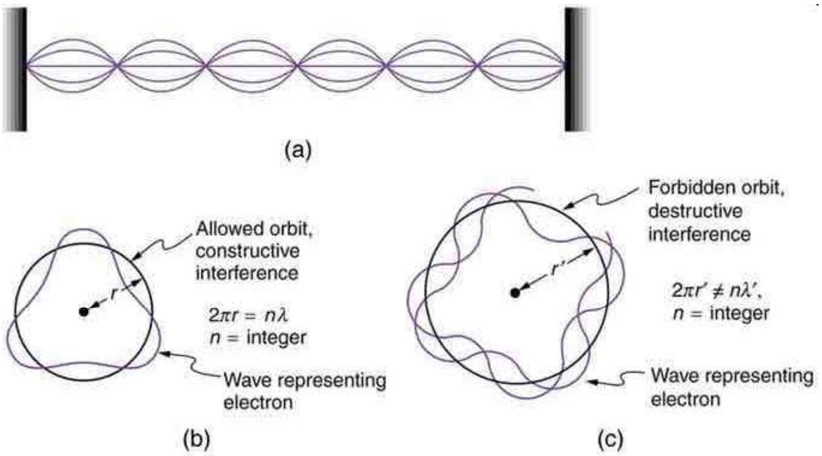


Figure 1.4 De Broglie Model of the atom. (a) electrons have wave and particle properties, specifically a wavelength, if the wavelenth when traced around an orbital results in (b) constructive interference the orbital is allowed and if it results in (c) destructive interference the orbital not allowed. This explains the quantitization of orbitals. credit: c: `http://oer2go.org/mods/en-boundless/www.boundless.com/physics/textbooks/boundless-physics-textbook/atomic-physics-29/the-early-atom-185/de-broglie-and-the-bohr-model-692-6303/index.html`

Model	Key Aspect
Rutherford	Nucleus is small, dense, positive charge.
Bohr	Electrons are in quanitized orbitals.
De Broglie	Electrons have properties of waves and particles
Quantum Mechanics	Electron orbitals have different shapes - s, p, d, f.

Table 1.2 Summary - Models of the Atom

1.2 Quantum Mechanic Model of the Atom

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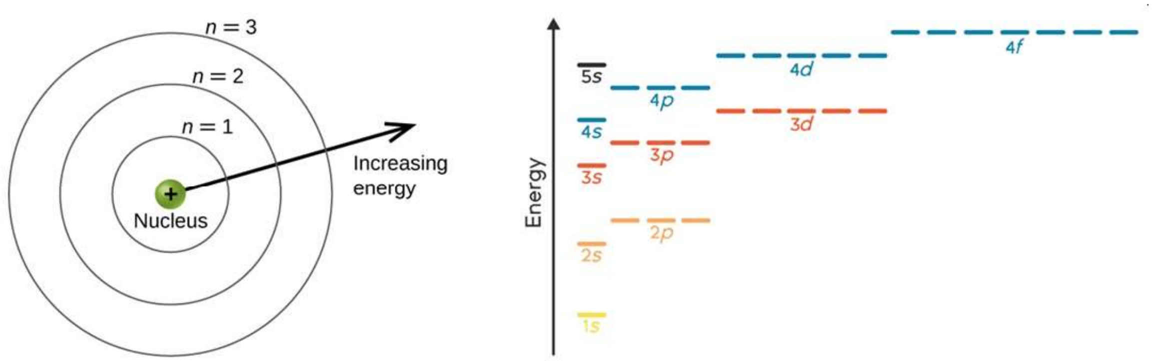
Quantum mechanics uses a mathematical wave-function to describe the location of electrons around an atom. Much like driving a car does not mean you can take one apart and put it back together, one can use Quantum Mechanics to describe electrons without understanding all of the mathematics behind it. Quantum mechanics describes the location of an electron using the four variable given in Table 1.3.

The **principal quantum number** (n) describes the distance an electron is from the nucleus. This also gives the energy of the electron according to Coulomb's Law which says the energy is inversely proportional

Name	**Symbol**	**Importance**
Principal	n	size and energy of (orbital or shell)
Angular Momentum	l	shape of orbital (4 allowed shapes - s,p,d,f)
Magnetic	m_l	orientation of orbital and # of sub-orbitals
Spin	m_2	electron spin - 2 allowed values (+ 1/2 or - 1/2)

Table 1.3 The Four Quantum Numbers, their commonly used symbols and what they describe about an electrons position around the nucleus.

to the distance from the nucleus. Electrons closer to the nucleus have a lower energy (more negative) energy than those further from the nucleus.



(a)

(b)

Figure 1.5 (a) The Principal quantum number (n) determines distance the orbital is from the nucleus which using Coulomb's law can also be considered an energy level. The closer to the nucleus the electron is the lower in energy the orbital is. (b) Energy level diagram showing relative energy, orbital shape, and number of suborbital.

The **angular momentum quantum number** (l) describes the shape of orbitals and is normally designated by a letter (s,p,d or f). Unlike the planetary orbitals from the Bohr model of the atom, quantum mechanics predicts more complicated shapes. s-orbitals are spherical in shape, p-orbitals are shaped like dumb-bells d-orbitals and f-orbitals are more complex as shown below in Figure1.6

The **magnetic quantum number** (m_l) describes the orientation in space of each orbital and the number of sub-orbitals in each level (n). For a spherical s-orbital there is a single orientation of the orbital. For the dumb-bell shaped p-orbitals there are three orientations, one along each axis, resulting in 3 separate orbitals. Orientations are noted by a subscript and the axis which the orbital is aligned. For the p-orbitals this results in a p_x, p_y, and p_z orbital. d and f-orbitals are more complex shapes and orientations which we can ignore except for noting that their are 5 d-orbitals and 7 f-orbitals. Figure1.6 show all of the orbital shapes and orientations.

The **spin quantum number** (m_s has two allowed values (+1/2 or -1/2) which also means that each sub-orbital can hold two electrons. Thus an s-orbital with 1 orientation can hold 2 electrons, p-orbitals with 3 orientations each holding 2 electrons holds a total of 6 electrons. d-orbitals hold 10 total electrons and f-orbitals hold 14 electrons. The spin associated with an electron is also important in Nuclear Magnetic Resonance (NMR) which is a technique used in organic chemistry to experimentally determine the structure of molecules.

Electrons are placed in different orbitals according to the Aufbau principals which state that (1) an orbital can hold two electrons (with opposite spin), (2) electrons always fill lower energy orbitals before higher energy orbitals and (3) electrons in degenerate orbitals fill singly and are spin aligned until forced to pair up. The energy level diagram on the right in Figure 1.5 shows the relative energy levels of the orbitals, though

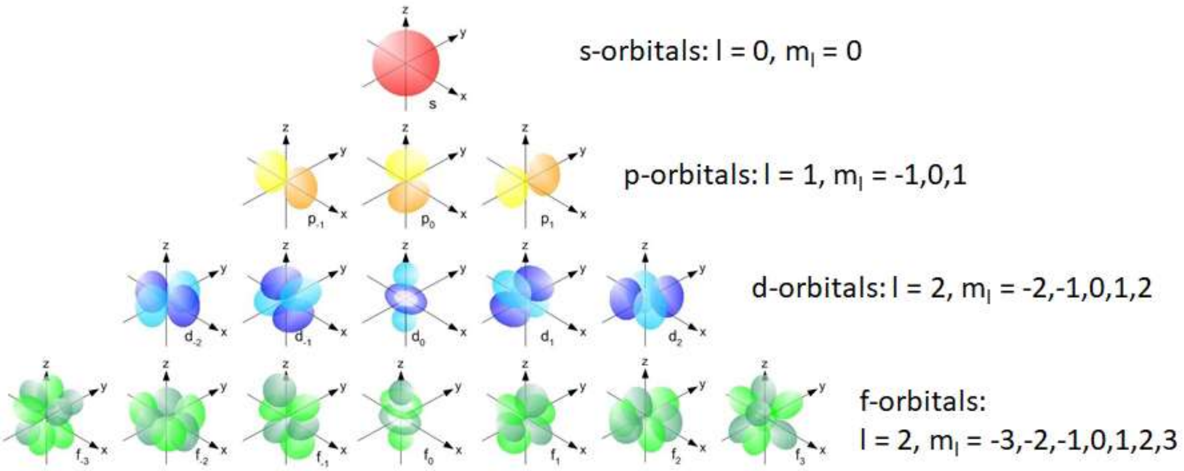
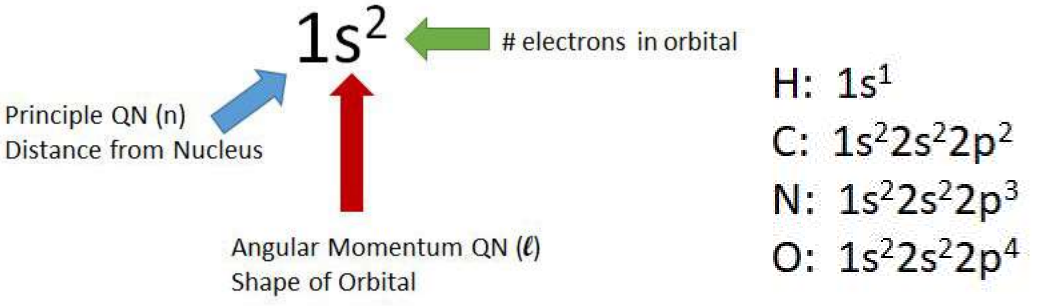


Figure 1.6 The angular momentum (l) quantum number determines the shape of orbitals described by the letters s, p, d, f. The magnetic (m_l) quantum number determines the number of orbitals (1, 3, 5, 7 respectively) and their orientation in space.

more frequently a condensed, shorthand notation is used in which only the principle quantum number, shape and number of electrons are shown.



(a) (b)

Figure 1.7 (a) Electron configuration notation used to show the energy levels of electrons in an atom. (b) Electron configurations for H, C, N, O - the four elements that are most important in organic chemistry. credit: author

The size and shape of the periodic table as shown in Figure 1.8 are reflected by the rules derived from quantum mechanics with the most important concepts being that the rows are related to the principle (n) quantum number, the width of each part of the periodic table reflects the number of electrons that are in a sub-orbital and the columns being associated with the atoms having the same electron configuration in the outermost orbital.

Valence electrons are those electrons found in the outer most orbitals s and p-orbital (orbital with the highest principle quantum number n) of an atom are easily gained or lost to make cations and anions which are attracted to each other by Coulomb's law to form ionic bonds. The same valance electrons can also be shared between atoms to form molecular compounds. Elements in the periodic table were initially placed on columns due to having similar chemical and physical properties, with the discovery of quantum mechanics, it is clear that elements in columns have the same number of valence electrons which is responsible for there similarities.

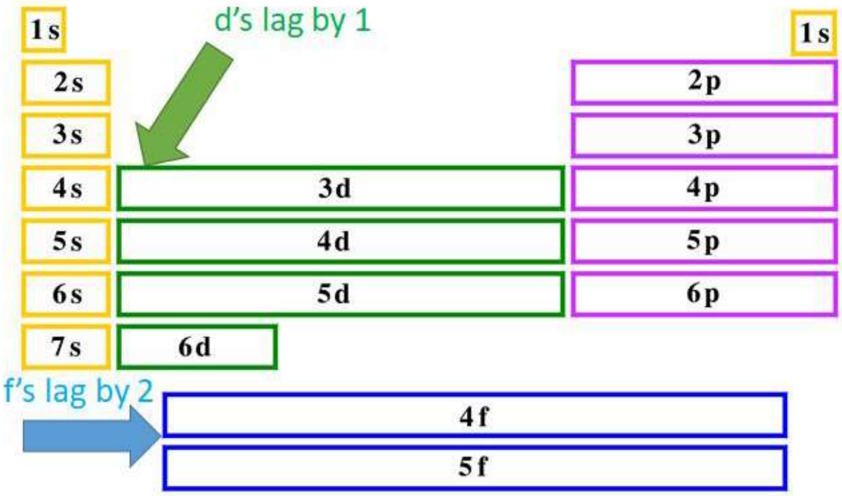


Figure 1.8 Relationship between the periodic table and quantum mechanics. Each row has the same principle (n) quantum number. The designation (s,p,d,f) determines the different sections with the width of each section determined by the number or orientation given by the angular momentum (l) quantum number with each orientation/sub-orbital holding two electrons.

1.3 Lewis Structures

Representing electrons using electron configurations is one way to illustrate what occurs, but another method has also proven quite useful which is commonly called Lewis structures. Gilbert Newton Lewis (1875-1946) developed a model about bonding between atoms to form molecules which he observed to occur such that the electrons in the valence shells add to eight. This is often called the **"octet" rule** and from our knowledge of quantum mechanics reflects having completing filled s and p orbitals (s^2p^6) which represents a stable state. The Lewis model is a simple, yet powerful, model of the atom which allows determination of molecular structure and geometry around a central atom. In most cases it is sufficient for our discussion of organic and biochemistry, though more advanced models based on quantum mechanics will also be examined.

Lewis electron dot structures or simply Lewis structures are a useful construct to keep track of valence electrons in representative elements. In this notation the valence electrons are represented by dots surrounding the atomic symbol of an element. Several examples are shown in Figure1.9. Ions are shown in brackets with the corresponding charge as a superscript.

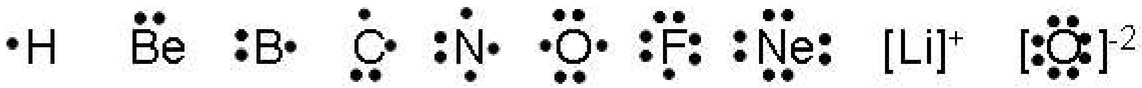


Figure 1.9 Lewis structure examples of the second row elements (Hydrogen to Neon), a cation (Lithium has lost its one valence electron), and an anion (Oxygen has gained two valence electrons). credit: author

Formation of Cations and Anions

Cations and anions form due to the stability gained from having an octet or s^2p^6 configuration in the atoms outermost orbital or valence shell. This explains the common charges that many elements have such as sodium always forming a +1 cation and chlorine always forming a -1 anion. Note that in Lewis structures only the outermost orbital is shown, so the empty outermost orbital around sodium is considered an octet.

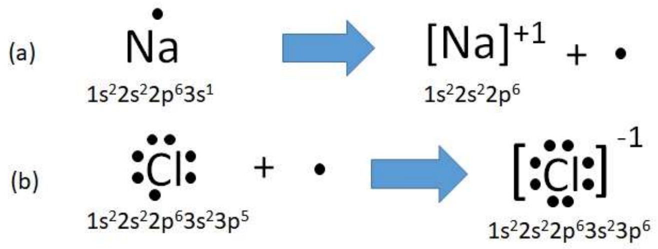


Figure 1.10 Formation of cations and anions using Lewis structures and electron configurations. (a) The sodium atom loses one electron in order to form a +1 sodium cation. (b) The chlorine atom gains one electron in order to form a -1 chlorine anion. Note that in Lewis Structures only the outermost orbital is shown, so the empty outermost orbital around sodium is considered an octet. credit: author

A general rule an which atoms tend to lose electrons (form anions) or gain electrons (form cations) to achieve an octet is an atoms location on the periodic table. The **metalloids** elements - Boron, Silicon, Germanium, Arsenic, Antimony, Tellurium and Polonium separate the **metals** (to the left) which form cations from the **non-metals** (to the right) which form anions. The exception to the rule being Hydrogen which completes an "octet" with two electrons (due to not having a p-orbital) and is considered a non-metal but typically forms a cation.

1.4 Ionic, Polar Covalent and Covalent Compounds

The **chemical bond** that occurs between atoms to form compounds or molecules minimizes the energy between the charged particles (protons in the nucleus and electron in orbitals) according to Coulomb's Law. It can occur in two ways, the formation of ionic bonds or the formation of molecular or covalent bonds. If two atoms can lose and gain electrons to complete octets an ionic bond forms between the cation (positive charge) and the anion (negative) charge. If two atoms share electrons to complete octets than a molecular or covalent bond forms due the shared electrons being attracted to protons in both atoms nuclei.

	Ionic Compounds	**Molecular Compounds**
Chemical Bond	Lose/Gain Electrons	Share Electrons
Formed between	metals/non-metals	non-metals/non-metals
Bond Strength	Strong	Weak
Structure	Lattice	Discrete Molecules

Figure 1.11 Key differences between Ionic and Molecular Compounds.

Ionic Compounds

Ionic compounds occur when cations (metals) and anions (non-metals) formed by losing and gaining electrons are then subsequently attracted to each other due to Coulomb's law. This can be shown using Lewis structures and electron configurations as shown in Figure 1.12. Ionic bonds occur between a full positive and full negative charge and are a strong attraction compared to molecular bonds which share electrons. Ionic compounds generally form lattice structures.

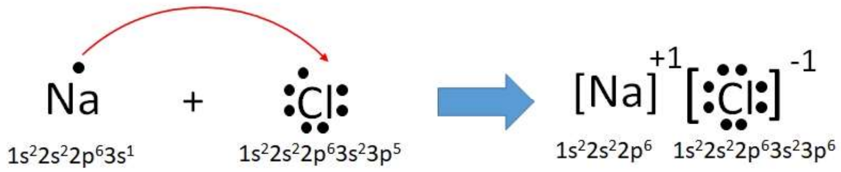


Figure 1.12 Formation of an ionic compound. The sodium atom loses one electron, to chlorine to complete both octets, the resulting cation and anion form an ionic bond due to Coulomb's law. credit: author

Molecular or Covalent Compounds

Molecular compounds (also commonly called **Covalent compounds**) occur when atoms can't form octets by gaining or losing electrons and instead must share electrons to form octets as shown in Figure 1.13. In Lewis Structures shared bonds can be represented in several ways though the most common is a line between two atoms represents a shared pair of electrons. The shared pair of electrons are counted towards each atoms octets.

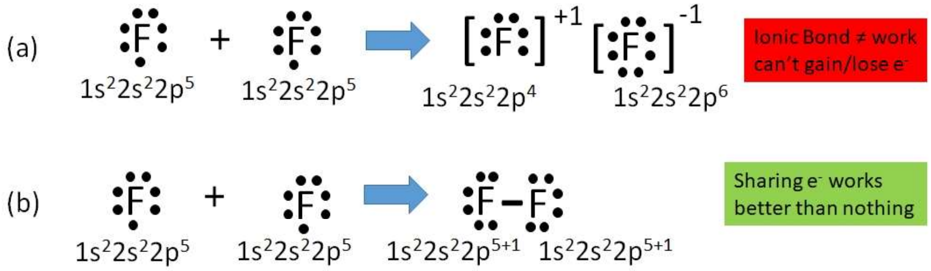


Figure 1.13 (a) Fluorine can't form an ionic bond with itself because only one atom can achieve an octet. (b) Fluorine forms a molecular compound by sharing a pair of electrons (the solid line represents two shared electrons) in order to complete both octets. credit: author

The energy is minimized when forming a molecular bond as the electrons feel the attractive force of both nuclei which reduces the overall energy of the system.

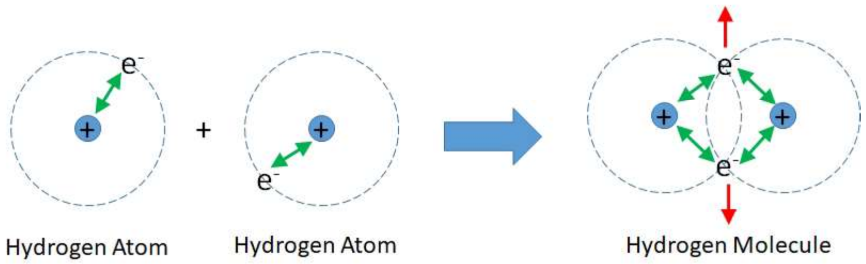


Figure 1.14 Formation of a molecular/covalent bond. On the left is two individual hydrogen atoms, the green arrows represent the attractive forces between the nucleus and the electron. On the right is a hydrogen molecule which allows both electrons to see both nuclei and increases the attractive forces. The red arrows represent electron-electron repulsion which also occur. The net effect is to lower the energy of the system. credit: author

Up to three pairs of electrons can be shared this way forming single (one shared pair of electrons), double (two shared pairs of electrons) and triple (three shared pairs) bonds. **Polyatomic ions** which are part ionic (gain or lose electrons) and part molecular (share electrons) can also be represented by Lewis Structures as a hybrid of both representations.

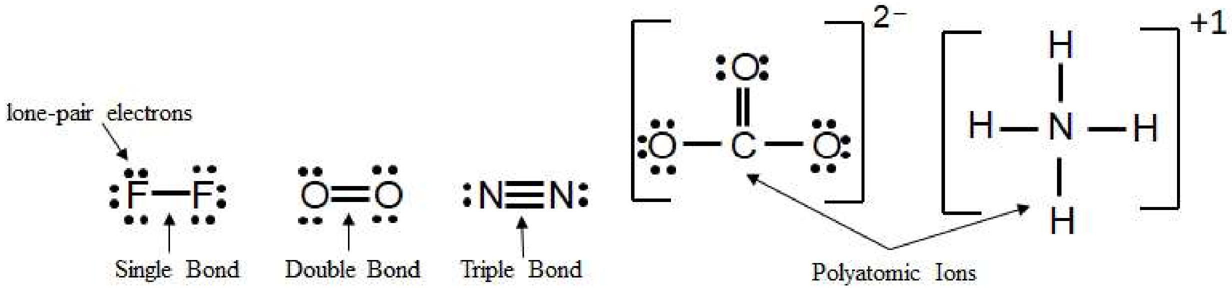
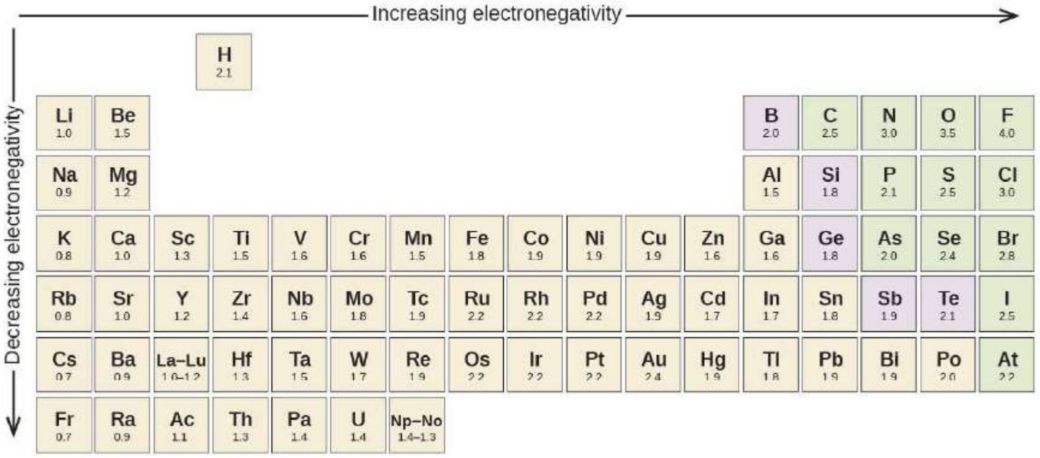


Figure 1.15 Lewis Structures illustrating single, double, triple bonds and polyatomic ions. credit: author

Electronegativity is the attractive force an atom has for the shared electrons in a bond. Electronegativity values are assigned to elements, and can be found in Figure 1.16. In general electronegativity increases across a row (Fluorine is the most electronegative element), and decreases down a column (Francium is the least electronegative element).



			H 2.1														
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La–Lu 1.0–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.2
Fr 0.7	Ra 0.9	Ac 1.1	Th 1.3	Pa 1.4	U 1.4	Np–No 1.4–1.3										

Figure 1.16 Electronegativity values for different elements. The larger the number, the more electronegative the element. credit: ??? (OER Book)

Bond Polarity describes the sharing of electrons between atoms. **Nonpolar Covalent** bonds form between atoms that are alike (ΔEN < 0.5), the shared electrons spend equal amounts of time around each atom and the electron density is symmetrical around the bond. **Polar Covalent** bonds occur between atoms that have different electonegativities ($0.5 < \Delta\text{EN} < 2.0$) which results in the electron density between the atoms being unsymmetrical around the bond. The resulting unsymmetrical distribution of electrons is indicated by using the Greek symbols δ^+ to indicate a small excess of positive charge, or δ^- to indicate a small excess of negative charge around an atom. The more electronegative element (larger value) is assigned the symbol (δ^-) the element with the smaller electronegativity value is assigned the symbol (δ^+). Another common method is to use a modified line for the bond with an arrow pointed towards the more electronegative atom, and a small cross towards the more electropositive atom. An example of both labeling methods is shown in Figure 1.17.

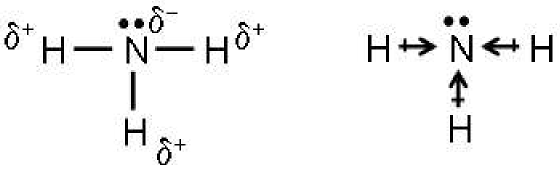


Figure 1.17 In polar bond the unsymmetrical distribution of electrons in a molecular bond between two atoms can be shown different ways. credit: author

In addition to bond polarity, **Molecular Polarity** can also occur when there is an unequal or unsymmetrical distribution of electron density around a molecule (not just between two atoms). **Nonpolar molecules** molecules have a symmetrical distribution of electron density around the entire molecule. **Polar or Dipolar** molecule has an unsymmetrical distribution of electrons around the molecule which results in the molecule being capable of interacting with each other like magnets due to Coulomb's law. The unsymmetrical distribution of electrons across a molecule also uses the (δ^+/δ^-) nomenclature though it is frequently shown pictorially as shown in Figure 1.17. Molecules with nonpolar bonds or with polar bonds that are symmetrical are always nonpolar whereas, molecules with polar bonds that are unsymmetrical are always polar.

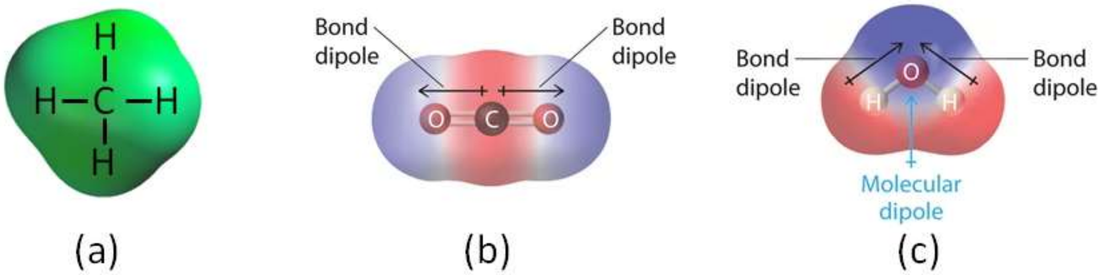


Figure 1.18 (a) A nonpolar molecule with nonpolar bonds and symmetrical distribution of electrons across the molecule. (b) A nonpolar molecule with polar bonds but a symmetrical distribution of electrons across the molecule (c) A polar or dipolar molecule with polar bonds and an unsymmetrical distribution of electrons around the atoms. credit: chemlibre + author

Summary of Ionic, Covalent and Polar Covalent Bonding

As has been discussed above there are three primary types of chemical bonds formed between atoms depending primarily on the electron configuration or Lewis structure and the electronegativity difference between the elements. These differences are summarized in Figure 1.20

As a general rule ionic bonds form when the Lewis structure can from octets by losing and gaining electrons, occurs between metals and non-metals and the elements have large differences in electronegativity ($2.0 < \Delta$EN). The ionic bond is between a full positive and negative charged cation and anion resulting a strong attraction due to Coulomb's law.

Molecular or covalent bonds form when the Lewis structure has to share electrons to complete octets, occurs between nonmetals and nonmetals and the elements have a small difference in electronegativity. The bond can be either nonpolar or polar. It is nonpolar if the electrons are shared relatively equally between the atoms due to a small difference in electronegativity (ΔEN < 0.5) between the two atoms. The bond is polar if the electrons are shared unequally between the atoms due to a intermediate difference in electronegativity ($< 0.5\ \Delta$EN < 2.0) between the atoms. The resulting chemical bond is generally weaker than an ionic bond because no fully positive or negative charges are produced.

	Nonpolar Covalent	Polar Covalent	Ionic
Form between:	nonmetals-nonmetals	nonmetals-nonmetals	metals-nonmetals
ΔEN:	0-0.5	0.2-2.0	2.0-4.0
Electrons are:	shared equally	shared unequally	lost and gained
Bond Strength:	Weaker	Weaker	Stronger
Structure:	Discrete Molecules	Discrete Molecules	Lattice

Figure 1.19 Key differences between nonpolar covalent, polar covalent bonds and ionic bonds.

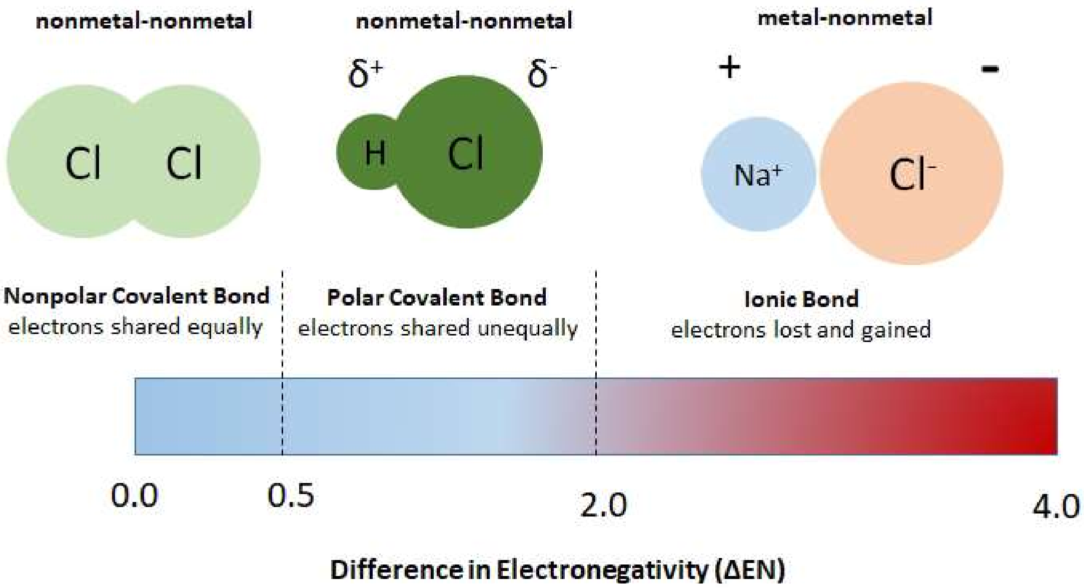


Figure 1.20 Key differences between nonpolar covalent, polar covalent bonds and ionic bonds. credit: author

1.5 Drawing Lewis Structures

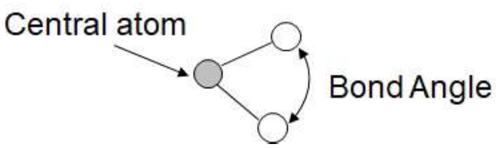
Molecular structure plays a crucial role in organic and biochemistry, the ability to draw Lewis structures, assign geometry, determine molecular polarity are one key to a better understanding of the topics. The following rules represent a good starting point for drawing Lewis structure, assigning geometry and determining the molecular polarity. A detailed example for two molecules is located at the end of this section.

1. Count the valence electrons in the molecule
2. Build a trial structure
3. Distribute electrons to complete octets
4. Finish incomplete octets by making single and double bonds
5. Determine the molecular geometry
6. Determine if the molecule is nonpolar or dipolar.

The geometry around each central atom in a molecule is uniquely determined by a combination of the number of atoms bonded to central atom and the number of lone pair electrons bonded to the central atom. Valence Shell Electron Pair Repulsion Theory (VESPR) states that atoms and lone pair electrons want to remain as far apart as possible due to the repulsive forces between electrons. This results in six primary shapes which obey the octet rule (violations of the octet rule are rare in organic and biochemistry, and will not be required knowledge). For larger molecules there may be more than one central atom and one geometry associated with the molecule. Figure 1.21 and 1.22 defines and gives examples for each geometry.

# atoms bonded	**# lone pairs**	**Geometry**	**Bond Angle**
4	0	Tetrahedral	109.5
3	1	Trigonal Pyramidal	109.5
2	2	Bent	109.5
3	0	Trigonal Planar	120
2	1	Bent	120
2	0	Linear	180

(a)



(b)

Figure 1.21 (a) Six geometries predicted by VSEPR theory. (b) A central atom must be connected to at least two other atoms in order to produce a geometry and bond angle credit: author

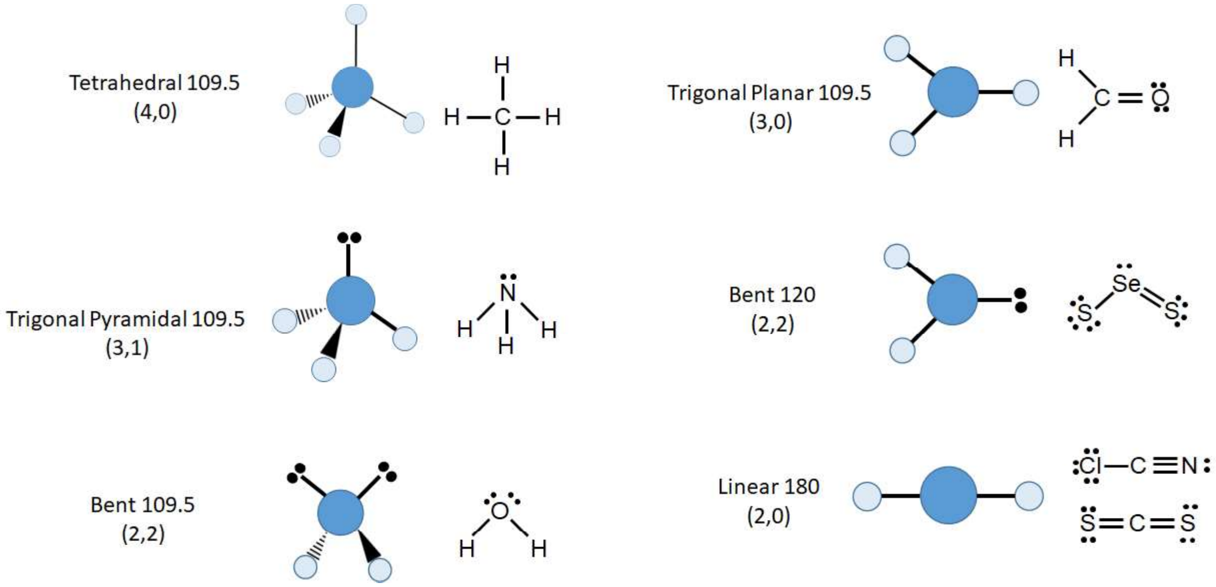


Figure 1.22 A 3D representation of each of the six geometries predicted by VSEPR theory and an example molecule with that geometry. Numbers in parenthesis represent the number of atoms bonded and the number of lone pairs which is unique for each geometry. credit: author

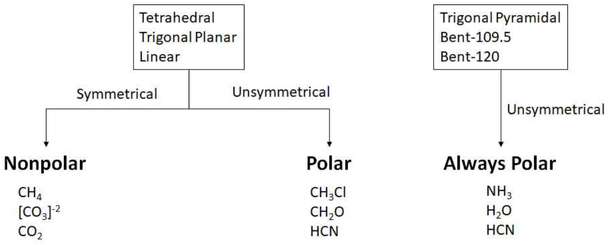
If the molecule is nonpolar or polar will determine how the molecules interact with other molecules and influences physical and chemical properties. More detail is in the next section on Intermolecular Forces (IMF's). In a nonpolar molecule the distribution of electrons around the molecule is symmetrical while in a polar molecule the distribution of electrons is asymmetrical resulting in a polarized molecule where one end has an excess of positive charge and is labeled δ^{+}) and one end has an excess of negative charge (δ^{-}). To determine the molecular polarity requires knowing the difference in electronegativity between the atoms (ΔEN) and the molecular geometry.

Organic compounds are mostly composed of C, H, N, and O, Figure 1.23 shows the most common bonds, the difference in electronegativity and whether the bond type is nonpolar or polar using the electronegativity values found in Figure 1.16. The predominant bond type in organic molecules C-H is nonpolar, with C-O, O-H and N-H bonds being very polar.

The geometry of a molecule is also used to determine the molecular polarity, symmetrically shaped molecules are nonpolar, any assymetrical distribution of electrons in a bond cancels out, while in unsymmetrical

Bond	ΔEN	Bond Polarity
C-H	0.4	nonpolar
C-N	0.5	slightly polar
O-N	0.5	slightly polar
N-H	0.9	polar
C-O	1.0	polar
O-H	1.4	polar

(a)



(b)

Figure 1.23 (a) Bond polarity for common organic bonds between C, H, N, and O. (b) Symmetrical geometries always result in nonpolar molecules, Unsymmetrical geometries can results in polar molecules. credit: author

molecules if a polar bond exists than the molecule will also be polar. Molecular geometry's that are symmetrical will be nonpolar if the surrounding atoms are identical whereas if the surrounding atoms are different the molecule will be polar. Any molecular geometry with a lone pair of electrons is unsymmetrical and will result in a polar molecule. There are four potential outcomes when combining bond polarity and molecular geometry are shown Figure 1.24.

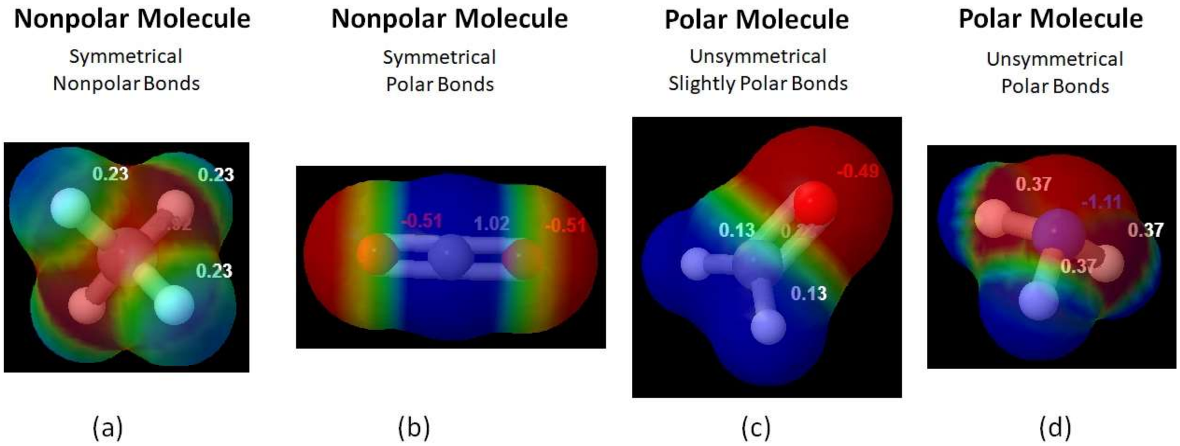


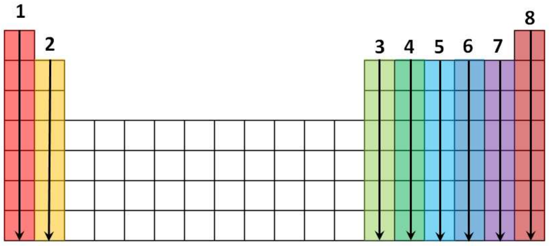
Figure 1.24 Four possible combinations of geometry and bond polarity resulting in nonpolar or polar molecules. Red indicates areas of excess positive charge, blue represents area's of excess negative charge. Values indicate relative amounts of excess charge (red = positive, white = negative). Models constructed using: `http://www.chemeddl.org/resources/models360/models.php`. credit: author

Step 1: Calculate the number of valence electrons

a. Add up valence electrons for all atoms

b. Cation - lose electrons; <u>subtract</u> the charge

c. Anions - gain electrons; <u>add</u> the charge



Ex: NH_4^+

N = 5
4 (H) = 4(1)
Charge = -1

Valence e^- = 8

Ex: CO_3^{-2}

C = 4
3 (O) = 3(6)
Charge = +2

Valence e^- = 24

Step 2: Build a trial structure

a. Place the least electronegative (EN) element in the middle

b. Arrange other atoms around it to make molecules as symmetrical as possible

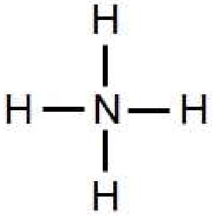
c. Draw one bond connecting atoms together

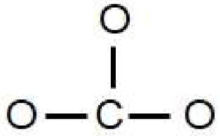
d. H makes 1 bond (never in middle)

e. F, Cl, Br, and I generally form 1 bond

f. Oxygen rarely bonds to oxygen

g. Typical Bonding Patterns – H = 1 bond , O = 1 or 2 bonds, C = 4 bonds, N = 1,2,3 and rarely 4 bonds if it is part of a polyatomic ion.





Step 3: Distribute electrons

a. Count the electrons left after making the trial structure

Remaining e- = Valence e- - 2 × (# of Bonds)

b. Distribute remaining electrons to complete octets (noble gas configurations)

c. Start with the most electronegative (EN) element first

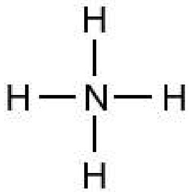
d. Remember H has an "octet" with 2 electrons

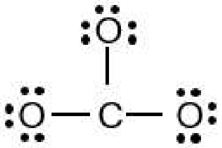
Valence e^- : 8
- 2 (# of Bonds): – 2·(4)

Remaining e^-: 0

Valence e^- : 24
- 2 (# of Bonds): – 2·(3)

Remaining e^-: 18



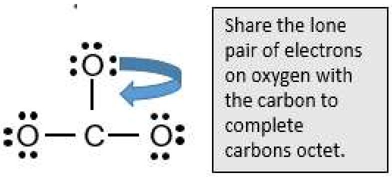


Step 4: Finish any incomplete octets by sharing electrons

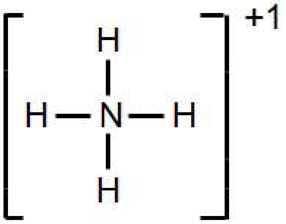
a. If some atoms can't complete octets remove unshared electron pairs and form double or triple bonds.

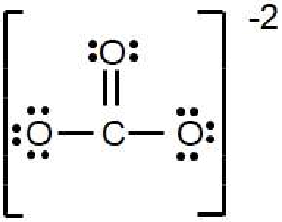
b. If all atoms have complete octets the Lewis structure is done

c. Remember to put cations and anions in brackets and include the charge



Share the lone pair of electrons on oxygen with the carbon to complete carbons octet.

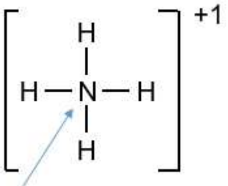




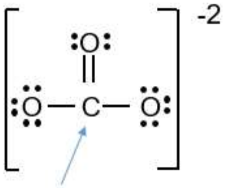
Step 5: Determine the geometry of each Lewis structure

a. Count the number of atoms bonded to the central atom and the number of lone pairs around each central atom.

b. Use Figure 1.21 to determine the geometry



4 atoms, 0 lone pair
Tetrahedral – 109.5



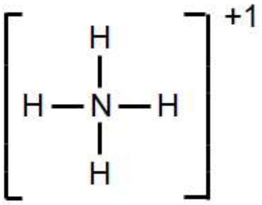
3 atoms, 0 lone pair
Trigonal Planar – 120

Step 6: Determine the polarity of the molecule

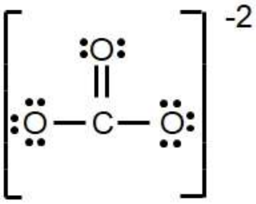
a. Refer to Figure 1.24

b. Nonpolar molecule - symmetrical or nonpolar bonds

c. Polar Molecule - unsymmetrical + polar bonds



Symmetrical
Nonpolar



Symmetrical
Nonpolar

1.6 Intermolecular Forces (IMF's)

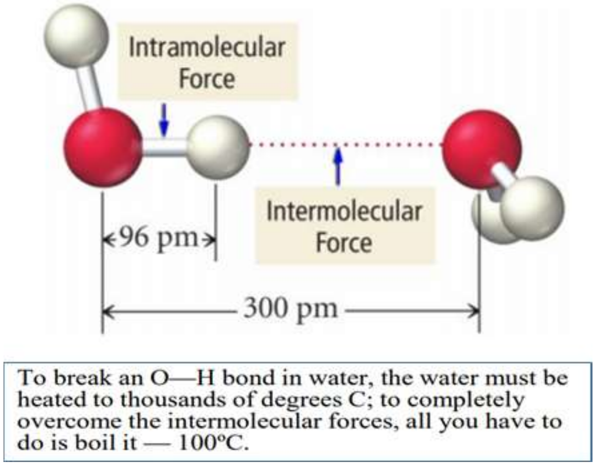
> While organic and biological chemistry is a very diverse field of study, one fundamental question that interests all organic chemists is how the structure of an organic molecule determines its physical properties. To understand why sperm oil has properties that made it both a useful industrial lubricant for humans and an effective buoyancy control and/or sonic lens for a hunting sperm whale, we first have to understand the nature of both the forces holding each wax molecule together – the covalent single and double bonds between atoms – and also the forces governing the noncovalent interactions between one wax molecule and all the others around it – the so-called 'intermolecular forces' which determine physical properties such as viscosity, melting point, and density.
>
> Soderberg

Chemical Bonds occur when electrons are gained or lost to form ionic bonds or shared between atoms to form molecular bonds. Chemical bonds are responsible for the chemical properties of a compound. Chemical bonds are a strong attractive force due to Coulomb's law, ionic bonds are very strong and occur between a cation (full + charge) and an anion (full - charge), while molecular bonds are strong and occur when atoms share electrons.

Intermolecular Forces (IMF's) occur between molecules and are responsible for the physical properties of molecules. Intermolecular forces are primarily due to Coulomb's law but are much weaker than a chemical bond as the attraction is between molecules with partial positive (δ^+) and negative (δ^-) charges due to the asymmetric distribution of electrons around the molecule.

	Chemical Bond	**Intermolecular Force's**
Between	atoms	molecules
Strength	Strong	Weak
Properties	Chemical	Physical
Types	Ionic	LDF
	Molecular	DD
		HB
		ID
Drawn as	Solid Line	Dashed Line

(a)



To break an O—H bond in water, the water must be heated to thousands of degrees C; to completely overcome the intermolecular forces, all you have to do is boil it — 100°C.

(b)

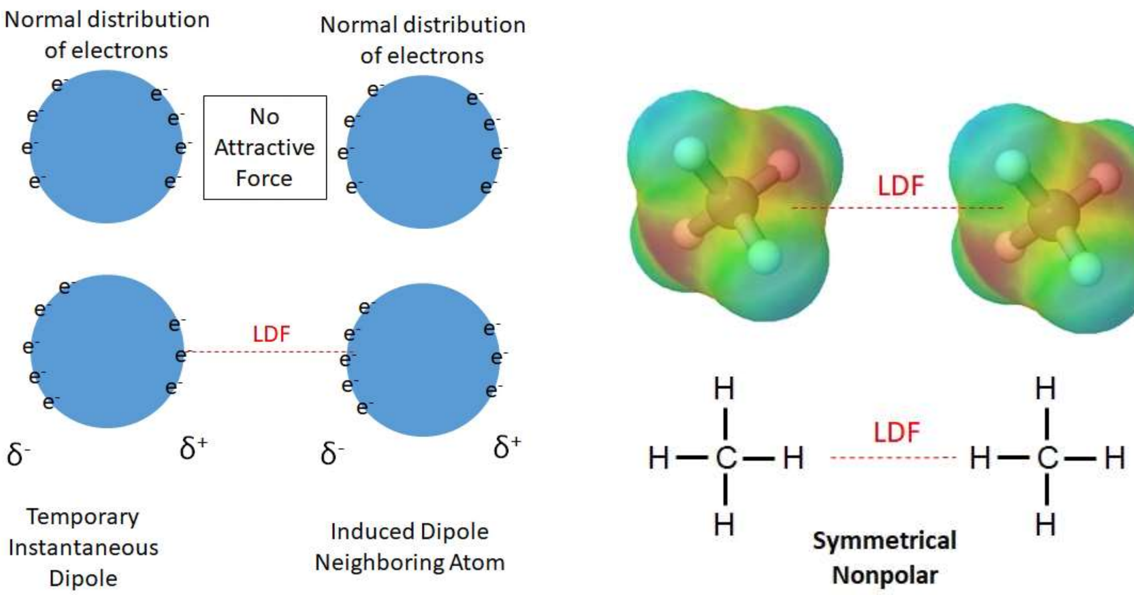
Figure 1.25 (a) Summary of the differences between chemical bonds and intermolecular forces. (b) Lewis structure showing the difference between a chemical bond and an intermolecular force. credit: unknown

London Dispersion Forces (LDF)

London Dispersion Forces (LDF's) also known as **Dispersion Forces** occur between nonpolar molecules due to the formation of temporary, instantaneous dipoles. These temporary dipoles form because the electrons around a molecule are constantly in motion, at some point even in nonpolar molecules there will be a instantaneous moment (like a snapshot of a movie) in which the normally symmetrical distribution of electrons will be unsymmetrically distributed. The resulting dipole can induce a similar, though opposite, distribution of electrons in a nearby molecule resulting in a small electrostatic attractive force between the molecules due to Coulomb's law. This is illustrated in Figure 1.26 between two atoms and between two molecules. The attractive force is very weak as the dipoles are only temporary, however, the attractive forces between two molecules is directly proportional to the size electron cloud around the molecule, becoming very large for large molecules. Often molecular weight is used as an estimate of the size of the molecule. Molecular shape also plays a role as will be seen later.

Dipole-Dipole(DD) Forces

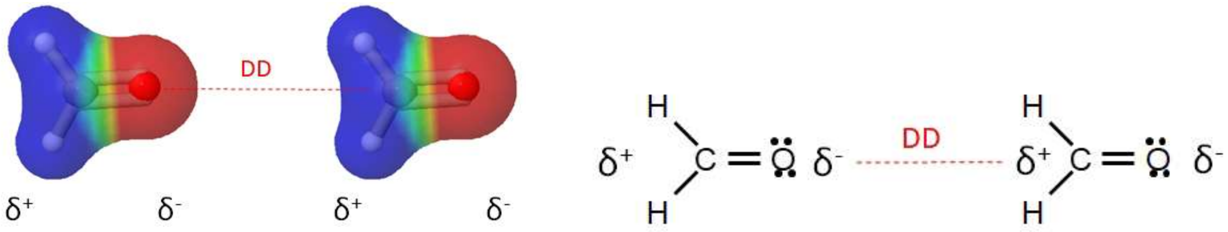
Dipole-Dipole attractions occur between two polar or dipolar molecules due to the electrostatic attraction between the partial charges. The attractive force is directly proportional to how assymetrically the electrons are distributed which can be approximated by the difference in electronegativity (ΔEN) between the atoms



(a) (b)

Figure 1.26 (a) Top: No attractive forces between nonpolar atoms. Bottom: Attractive force between two atoms due to temporary instantaneous dipoles creating a very small difference in the electron distribution. (b) London Dispersion forces between two different representations of methane (CH_4). Methane model constructed using: `http://www.chemeddl.org/resources/models360/models.php` credit: author

in the molecule or more formally by calculating the dipole moment (beyond the scope of this class). Dipole-Dipole attractions are slightly stronger than London Dispersion Forces. Figure 1.27 illustrates a dipole-dipole attraction between two methanal molecules (CH_2O also known as formaldehyde).



(a) (b)

Figure 1.27 (a) Dipole-Dipole attraction between two methanal (CH_2O) molecules showing the electron density. Methanal model constructed using: `http://www.chemeddl.org/resources/models360/models.php` (b) Dipole-Dipole interaction shown using Lewis structures. credit: author

Hydrogen Bonding (HB)

Hydrogen Bonding is a special case of dipole-dipole interactions that is considerably stronger due to Hydrogen only having one electron, resulting in any dipoles being significantly larger than for other atoms. For a Hydrogen Bond to occur Hydrogen must be bonded to a small highly electronnegative atom (Oxygen, Nitrogen or Fluorine) producing a large dipole due to the combination of hydrogen having a single electron and oxygen, nitrogen and fluorine producing a very polar bond. The hydrogen atom is attracted to a lone pair of electrons on another molecule or to a partial negative charge (δ^-) on another molecule. The resulting electrostatic attraction is approximately ten times stronger than a normal dipole-dipole attraction. The most common source of hydrogen bonding is of course water (H_2O) which can form two hydrogen bonds. Figure 1.28 illustrates this for several molecules. The term Hydrogen Bond is misleading, it is an intermolecular force (IMF), not a chemical bond.

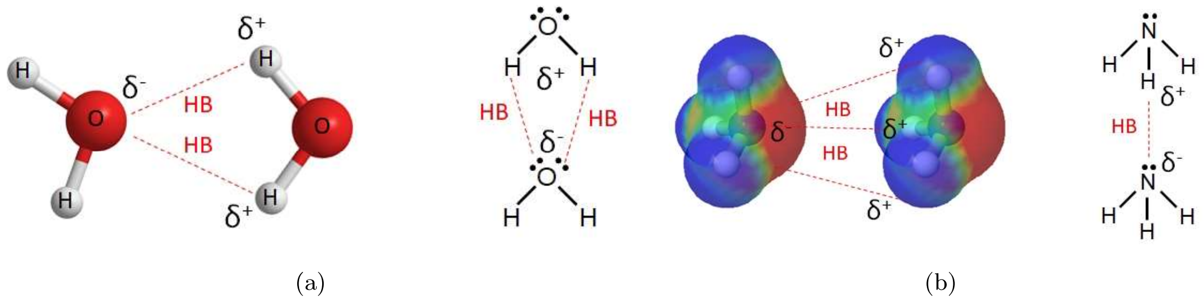


Figure 1.28 (a) Hydrogen bonding between two water molecules (H_2O). (b) Hydrogen bonding between two ammonia molecules (NH_3). Ammonia model constructed using: `http://www.chemeddl.org/resources/models360/models.php` credit: author

Ion-Dipole (ID)

Ion-Dipole (ID) interactions occur between an ion (cation or anion) and a dipolar molecule. The resulting electrostatic attraction between a full charge (+/-) and a partial charge (δ^+/δ^-) is the strongest intermolecular force. It is proportional to the charge on the ions and the size of the dipole moment, both of which will be ignored in this course.

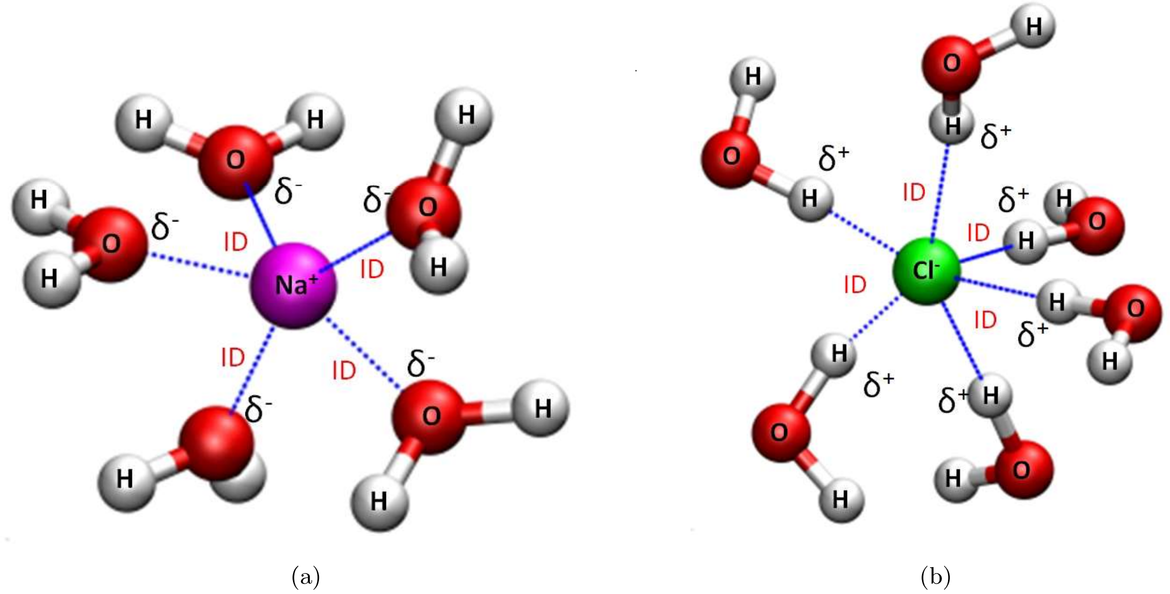


Figure 1.29 (a) Ion-Dipole attraction (blue dotted line) between a cation (Na^+) and water molecules (H_2O), note that the water molecules orient with the oxygen (δ^-) towards the cation. (b)Ion-Dipole attraction (blue dotted line) between an anion (Cl^-) and water molecules (H_2O), note that the water molecules orient with the hydrogen (δ^+) towards the anion. credit: author

Summary - Chemical Bonds and Intermolecular Forces

The relative strengths of chemical bonds intermolecular forces can vary greatly depending on the atoms bonded and molecular geometry. Figure 1.30 provides a brief summary of the forces and provides some numbers to give the reader a relative idea of how they compare.

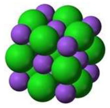
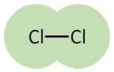
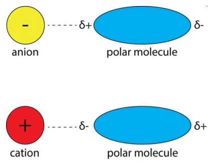
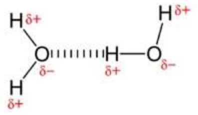
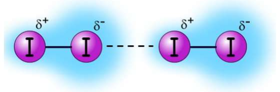
Interaction	**Attraction between**	**Strength kJ/mol**	**Model**	**Example Compound**
Ionic Bond	Cation-Anion	400-4000		NaCl, $Mg(NO_3)_3$
Molecular Bond	Atoms share e^-	150-1100		Cl_2, CH_4
Ion-Dipole (ID)	Cation and Polar Molec. Anion and Polar Molec.	40-600		$Na^+ \cdots H_2O$ $Cl^- \cdots H_2O$
Hydrogen Bond (HB)	H bonded to O, N, F attracted to lone pair e^-	10-40		$H_2O \cdots H_2O$
Dipole-Dipole (DD)	2 polar molecules	2-25 $\propto$ ΔEN		$HCl \cdots HCl$
London Dispersion Forces (LDF)	2 nonpolar molecules	0.05-40 $\propto$ Size		$I_2 \cdots I_2$

Figure 1.30 Summary of Attractive Forces between atoms (ionic and chemical bonds) and between molecules (intermolecular forces - ID, HD, DD, LDF). credit: NaCl - `https://commons.wikimedia.org/wiki/File:Sodium-chloride-unit-cell-3D-ionic.png`, Cl_2 - Author, Ion-Dipole - `https://www.ck12.org/book/ck-12-chemistry-basic/section/9.4/` Dipole-Dipole - `https://en.wikipedia.org/wiki/File:Dipole-dipole-interaction-in-HCl-2D.png`, London Dispersion Forces - `www.dlt.ncssm.edu`

1.7 Physical Properties and Intermolecular Forces

Physical properties of molecules are inherent characteristics of a molecule that can be determined without changing its composition (ie breaking and making chemical bonds) and are determined by the intermolecular forces between molecules. Physical properties include easily measured properties like melting points, boiling points, states of matters (solid, liquid, gas), density, solubility, vapor pressure and harder to measure properties such as color, taste and odor.