TERMS

- Anion - A negatively charged ion.
- Bond - That which holds together atoms in molecules and ions in lattices.
- Cation - A positively charged ion.
- Coulomb's Law - A mathematical formula whose consequence is that negatively and positively charged particles attract each other and similarly charged species repel each other.
- Covalent Bond - A bond that results from a sharing of electrons between nuclei.
- Ion - A charged species created by the gain or loss of an electron from an atom or neutral molecule.
- Ionic Bond - A bond that results from electrostatic attraction between oppositely charged ions. The cation is positively charged, while the anion is negatively charged.
- Lattice - A regularly repeating three-dimensional array of atoms, molecules, or ions.
- Molecular Orbital - A combination of atomic orbitals in molecular orbital theory that provides an orbital description of a molecule analogous to the atomic orbital description of atoms.
- Molecular Orbital Theory - A description of bonding that combines atomic orbitals from each bonded atom to produce a set of molecular orbitals.
- Molecule - A chemical species containing a covalent bond.
- Valence Shell Electron Pair Repulsion Theory - A theory used to predict bonding geometries that states that electron pairs will be distributed about the central atom to minimize electron pair repulsions.
DEFINITION

- Chemical reactions involve the making and breaking of bonds.
- To understand bonds, we will first describe several of their properties.
- The bond strength tells us how hard it is to break a bond.
- Bond lengths give us valuable structural information about the positions of the atomic nuclei.
- Bond dipoles inform us about the electron distribution around the two bonded atoms.
- From bond dipoles we may derive electronegativity data useful for predicting the bond dipoles of bonds that may have never been made before.
From these properties of bonds we will see that there are two fundamental types of bonds:

- Covalent, and
- Ionic.
Covalent bonding represents a situation of about equal sharing of the electrons between nuclei in the bond.

Covalent bonds are formed between atoms of approximately equal electronegativity.

Because each atom has near equal pull for the electrons in the bond, the electrons are not completely transferred from one atom to another.
IONSIC BONDING

- When the difference in electronegativity between the two atoms in a bond is large, the more electronegative atom can strip an electron off of the less electronegative one to form a negatively charged anion and a positively charged cation.

- The two ions are held together in an ionic bond because the oppositely charged ions attract each other as described by Coulomb's Law.
IONS VS. COVALENT

- Ionic compounds, when in the solid state, can be described as ionic lattices whose shapes are dictated by the need to place oppositely charged ions close to each other and similarly charged ions as far apart as possible.

- Though there is some structural diversity in ionic compounds, covalent compounds present us with a world of structural possibilities.

- From simple linear molecules like H₂ to complex chains of atoms like butane (CH₃CH₂CH₂CH₃), covalent molecules can take on many shapes.
When a highly electronegative atom and an electropositive one are bonded together, an electron is transferred from the electropositive atom to the electronegative atom to form a cation and an anion, respectively.

The cation, being a positively charged ion, is attracted to the negatively charged anion as described by Coulomb's law:
COULOMB’S LAW

\[ E = \frac{kQ_1Q_2}{R} \]
THE IONIC BOND

- A negative energy means there is an attractive interaction between the particles in the above expression.
- If the charges on the two ions are opposite in sign, they will attract each other.
- Conversely, if two charges are similar, they repel each other. Using this knowledge we can construct a graph of energy versus distance for two oppositely charges ions.
- At large distances, there is a negligible energy of attraction between the two ions, but as they are brought closer together, they are attracted to one another.
- Coulomb's law may seem to predict that the ions should be as close as possible to achieve a minimal energy state.
- However, the graph of energy versus distance shows that the ions are actually repelled at small distances.
- To explain this observation, remember that the ions' nuclei are both positively charged.
- When the nuclei approach each other, they repel strongly—accounting for the steep rise in potential as the ions get closer than the bond length.
- The depth (y-axis) of the minimum in the potential energy curve above represents the bond strength, and the distance (x-axis) at the energy minimum is the bond length.
- Using Coulomb's law and the bond length, one can actually predict with some accuracy the strength of an ionic bond.
- Performing a series of these calculations you find that ionic compounds formed by ions with larger charges create stronger bonds and that ionic compounds with shorter bond lengths form stronger bonds.
Ionic compounds do not usually exist as isolated molecules, such as LiCl, but as a part of a crystal lattice—a three dimensional regular array of cations and anions.

Ionic compounds form lattices due to the contributing coulombic attractions of having each cation surrounded by several anions and each anion surrounded by several anions.
An example of a crystal lattice is shown:

As you can see in the above figure, each lithium ion is surrounded by six chlorine atoms and vice versa. By virtue of the arrangement of the ions in the lattice, the lattice is lower in energy than it would be if the ions were separated into isolated LiCl molecules.
Using your knowledge of electronegativity, tell whether each of the following bonds will be ionic.

a. H-H
b. O-Cl
c. Na-F
d. C-N
e. Cs-F
f. Zn-Cl
PROBLEM # 2

- For each pair, indicate which bond will be stronger.
  a. C-H, Li-F
  b. Li-F, Mg-O
  c. Li-F, Cs-I
ANSWERS

- Problem # 1: c, e, f.
- Problem # 2:
  a. Li-F is stronger because it is an ionic bond while C-H is a covalent bond.
  b. Mg-O is stronger because Mg is charged 2+ and O is charged 2- while each ion in Li-F has only a charge of magnitude 1. Ions with higher charges are more strongly bound.
  c. Li-F is stronger than Cs-I because the Li-F bond is far shorter than the Cs-I bond. By Coulomb's law, shorter ionic bonds should be stronger.
COVALENT BONDS

- A covalent bond represents a shared electron pair between nuclei.
- The stability of covalent bonds is due to the build-up of electron density between the nuclei.
- Using Coulomb's law (discussed in Ionic Bonding), you should note that it is more stable for electrons to be shared between nuclei than to be near only one nucleus.
- Also, by sharing electron pairs nuclei can achieve octets of electrons in their valence shells, which leads to greater stability.
To keep track of the number and location of valence electrons in an atom or molecule, G. N. Lewis developed Lewis structures. A Lewis structure only counts valence electrons because these are the only ones involved in bonding. To calculate the number of valence electrons, write out the electron configuration of the atom and count up the number of electrons in the highest principle quantum number. The number of valence electrons for neutral atoms equals the group number from the periodic table. Each valence electron is represented by a dot next to the symbol for the atom. Because atoms strive to achieve a full octet of electrons, we place two electrons on each of the four sides of the atomic symbol. Some examples of Lewis structures for atoms are shown in the next slide.
We can create bonds by having two atoms come together to share an electron pair.

A bonding pair of electrons is distinguished from a non-bonding pair by using a line between the two atoms to represent a bond, as in the figure below.

A lone pair is what we call two non-bonding electrons localized on a particular atom.
EXAMPLE # 1

- You should note that each atom in the H-Br molecule has a full valence shell.
- Both the hydrogen and the bromine can count the two electrons in the bond as its own because the electrons are shared between both atoms.
- Hydrogen needs only two electrons to fill its valence, which it gets through the covalent bond.
- The bromine has an octet because it has two electrons from the H-Br bond and six more electrons, two in each lone pair on Br.
EXAMPLE # 2

- The deadly gas carbon monoxide, CO, provides an interesting example of how to draw Lewis structures.
- Carbon has four electrons and oxygen has six. If only one bond were to be formed between C and O, carbon would have five electrons and oxygen 7.
A single bond here does not lead to an octet on either atom.

Therefore, we propose that more than one bond can be formed between carbon and oxygen so that we can give each atom an octet of electrons.

To complete the carbon and oxygen octets in CO, we must employ a triple bond, denoted by three lines joining the C and O atoms as shown in the figure.

A triple bond means that there are six electrons shared between carbon and oxygen.

Such multiple bonds must be employed to explain the bonding in many molecules.

However, only single, double, and triple bonds are commonly encountered.
FORMAL CHARGE

When trying to draw the Lewis structures of charged molecules like NO$_2^-$, we encounter the problem of trying to tell where the negative charge is located. Is it on nitrogen or on one of the oxygens?

To combat these troubles, chemists have devised the notion of formal charge.

Using the Lewis structure and the rules for assigning formal charges, we can assign a formal charge to each atom in a Lewis structure to determine where the charges are located.