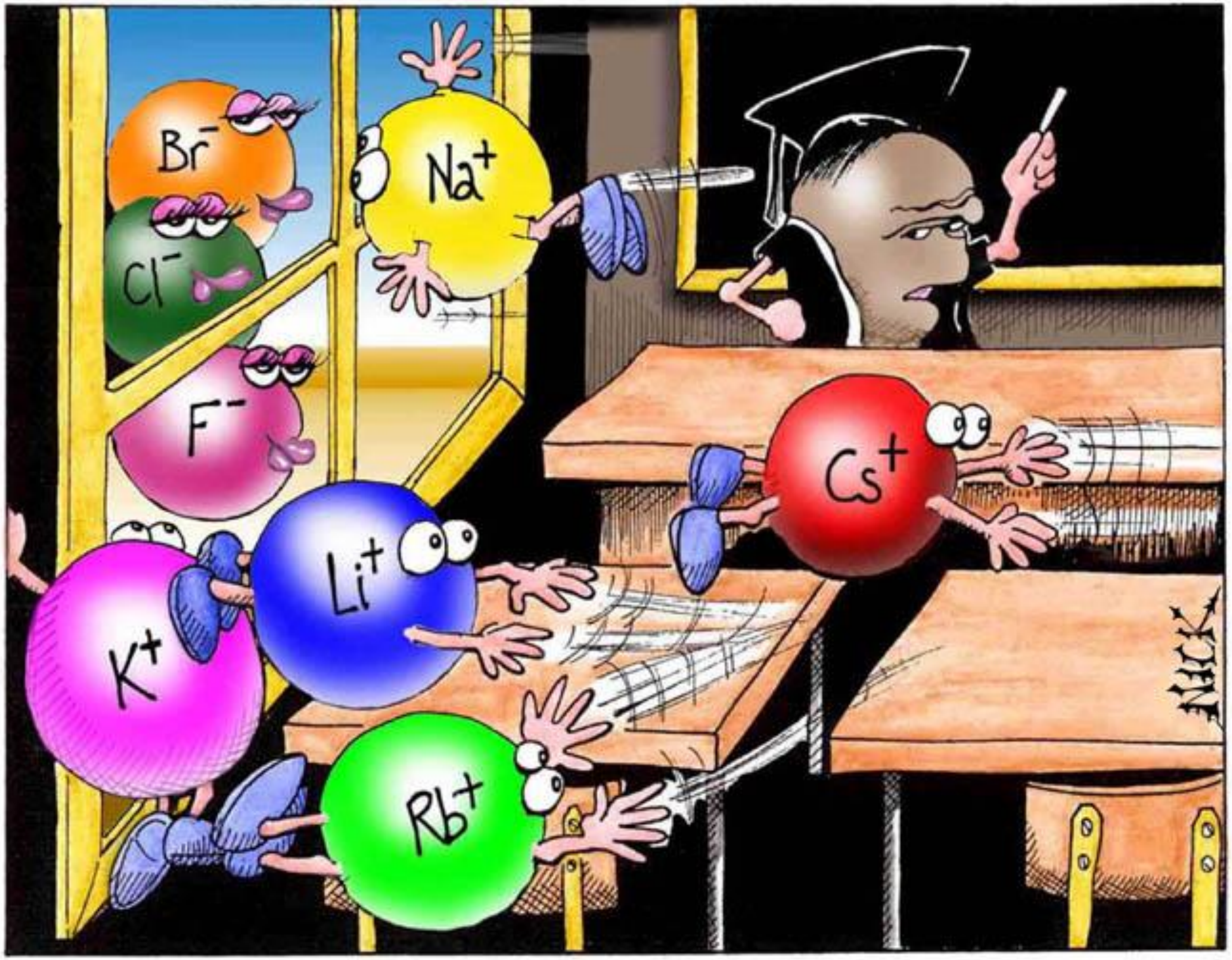
Chemical Bonding and Molecular Structure



"Perhaps one of you gentlemen would mind telling me just what it is outside the window that you find so attractive..?"

Cartoon courtesy of NearingZero.net

Big Ideas in Unit 6

- How do atoms form chemical bonds ?
- How does the type of a chemical bond influence a compounds physical and chemical properties?
- How do you name chemical formulas?
- How can we generate chemical formulas?

For Review: What are atoms?

- Smallest particle of an element that has all the characteristics of the element "building blocks" of all matter
- Can combine with other atoms to form compounds
- Most want to achieve an octet (8 valence electrons) can be done by giving, taking, or sharing valence electrons

Compounds- a substance formed when atoms chemically combine

- **When atoms form compounds they completely lose their identity**

In a Direct Union (Synthesis), as in all reactions, the reactants lose their properties and a NEW substance with different properties forms!!!!

Sodium Metal + Chlorine Gas → Sodium Chloride

Silver Metal

+

Poisonous Green Gas

→

White Crystal

Law of Definite Proportions

- Chemical compound contains the same elements in exactly the same proportions by mass regardless of sample size or source of substance
- 1700's Joseph Proust

- We all know the chemical formula for water is H_2O . It is essential for the body. The water from a Poland Spring bottle and from a your tap at home is always 2 hydrogen atoms to 1 oxygen atom

Law of Multiple Proportions

- Two elements may combine in different ratios to form different compounds.
- Change the ratio …Change the compound
- John Dalton

- Water is composed of hydrogen and oxygen in a 2 to 1 ratio needed for body
- Hydrogen Peroxide is H_2O_2 in a ratio of 2 to 2. Used as an antiseptic poisonous to body

Chemical Bonds

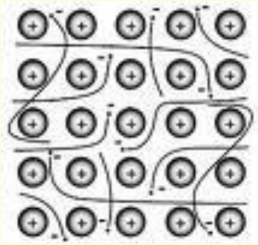
- Forces that hold groups of atoms together and make them function as a unit.

3 Major Types:

- Ionic bonds – transfer of electrons from metallic element to nonmetallic element
- Covalent bonds – sharing of electron pair between two atoms
- Metallic- de-localized electrons shared among metals

- Type of chemical bond will determine the physical and chemical properties of the substance
- All chemical bonds result from obtaining a full outer shell of electrons.

Metallic Bonding

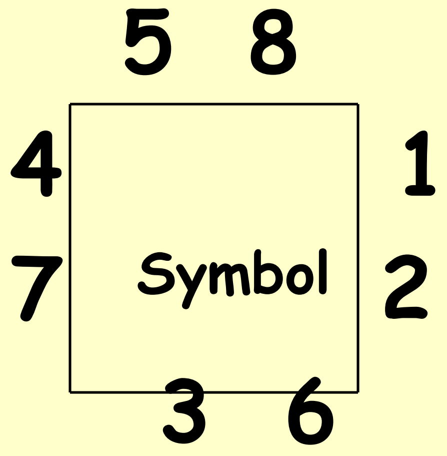


- The chemical bonding that results from the attraction between metal atoms and the surrounding sea of electrons (Copper, iron, aluminum)

- Vacant *p* and *d* orbitals in metal's outer energy levels overlap, and allow outer e to be shared among all nuclei

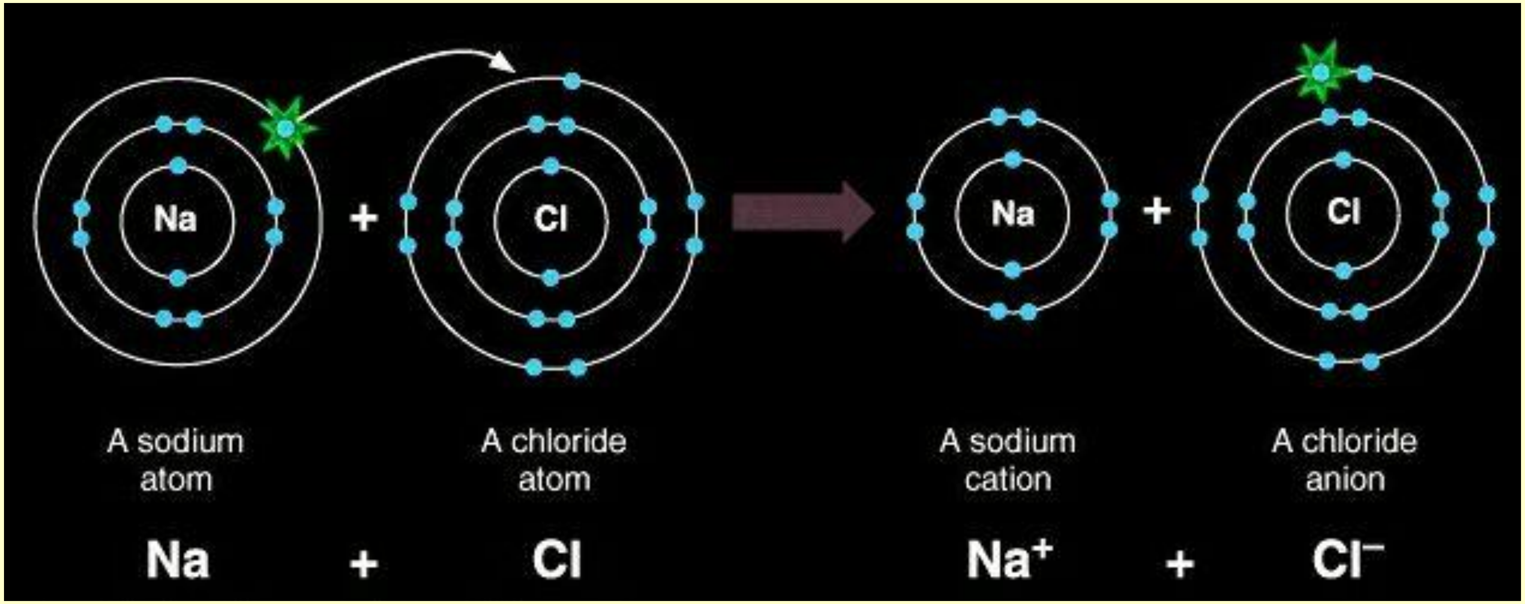
Electrons are constantly moving gives properties of conductivity and flexibility

Lewis Dot Diagrams- Show the kernal (inside of the atom..nucleus and inner shells) of the atom as the symbol and the valence electrons as dots



The Octet Rule – Ionic Compounds

Ionic compounds tend to form so that each atom, by <u>gaining or losing</u> electrons, has an octet of electrons in its highest occupied energy level.



Ionic Bonding: The Formation of Sodium Chloride

- Sodium has 1 valence electron
- Chlorine has 7 valence electrons
- An electron transferred from sodium to chlorine gives each an octet

Na $1s^2 2s^2 2p^6 \mathbf{3s^1}$

Cl $1s^2 2s^2 2p^6 3s^2 \mathbf{3p^5}$

Ionic Bonding: The Formation of Sodium Chloride

This transfer forms **ions, each with an <u>octet</u>:**

Cation→ Na^+ $1s^2\boxed{2s^22p^6}$

Anion→ Cl^- $1s^22s^22p^6\boxed{\mathbf{3s^23p^6}}$

When ionic bonds occur, metals are oxidized and non-metals are reduced

- Oxidation- Loss of electron(s)

(metallic element)

- $Na \rightarrow Na^{+} + 1\ e^{-}$

- Reduction- Gain of electron(s)

(non-metallic element)

- $Cl + 1\ e- \rightarrow Cl^{-1}$

Ionic Bonding:
The Formation of Sodium Chloride

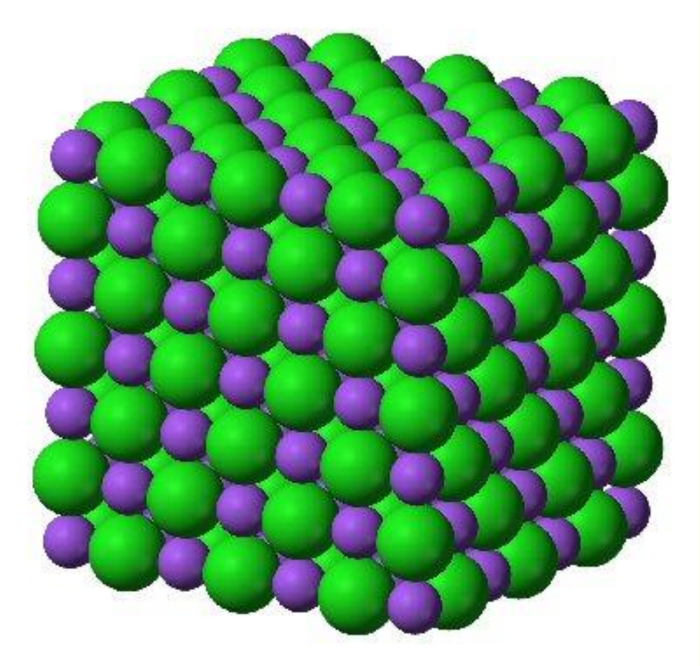
The resulting ions come together due to electrostatic attraction (opposites attract) and are held together tightly:

$Na^+ Cl^-$

The net charge on the compound must equal zero

Lattice Energy

- The energy given off when oppositely charged ions in the gas phase come together to form a solid.
- Can judge strength of bond
- Highly Negative= Strong Attraction



Up Close with Lattice energy

As you move down a group, lattice energy decreases.

WHY? - The atomic radius increases as you move down a group. Since the square of the distance is inversely proportional to the force of attraction, lattice energy decreases as the atomic radius increases.

Across a period

2) As you increase the magnitude of the charge (becomes more positive or more negative), lattice energy increases.

WHY? - The product of the charges of the particles is directly proportional to the force of attraction. Therefore, lattice energy increases as the charges increase.

Up Close with Lattice energy

Lattice Energies of Alkali Metals with Halides (kJ/mol)

	F^-	Cl^-	Br^-	I^-
Li^+	1036	853	807	757
Na^+	923	787	747	704
K^+	821	715	682	649
Rb^+	785	689	660	630
Cs^+	740	659	631	604

Lattice Energies of Salts of OH^- and O^{2-} with Cations of varying charge (kJ/mol)

	OH^-	O^{2-}
Na^+	900	2481
Mg^{2+}	3006	3791
Al^{3+}	5627	15916

Properties of Ionic Compounds

Phase:	Crystalline solids
IPF	High
Melting point:	Generally high
Boiling Point:	Generally high
Electrical Conductivity:	Excellent conductors, molten and aqueous
Solubility in H_2O	Generally Quite Soluble
Volatility (ability to evaporate)	Low

Lattice energy and properties

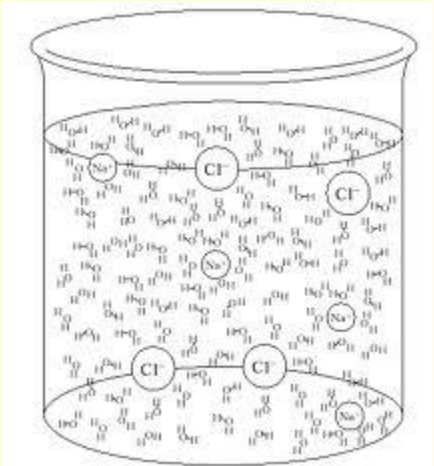
The higher the lattice energy the stronger the bond

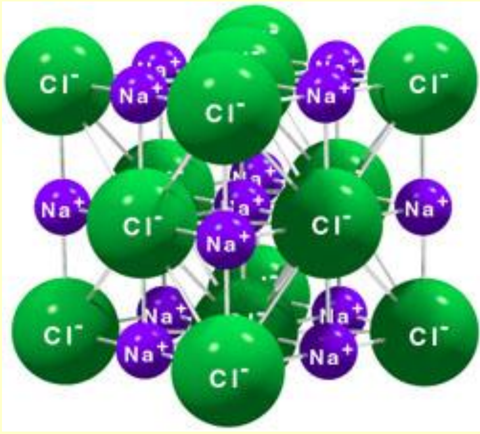
The higher the lattice energy the higher the melting point

The higher the lattice energy the lower the solubility

Properties of ionic compounds

- Exist as a crystal lattice structure
  - These are three dimensional arrays or crystals made up of ions in some sort of repeating pattern
    - The repeating pattern represents the simplest ratio of ions in the crystal and this is called its formula unit.
- All pure ionic substances are solids at room temperature
- Very high boiling and melting points
- When dissolved in water, ions dissociate; that is they break up into free ions in solution.
  - Ions are held in solution by their attraction to water
- Molten ionic solids and aqueous ionic solutions are capable of conducting electricity which means they are electrolytes.

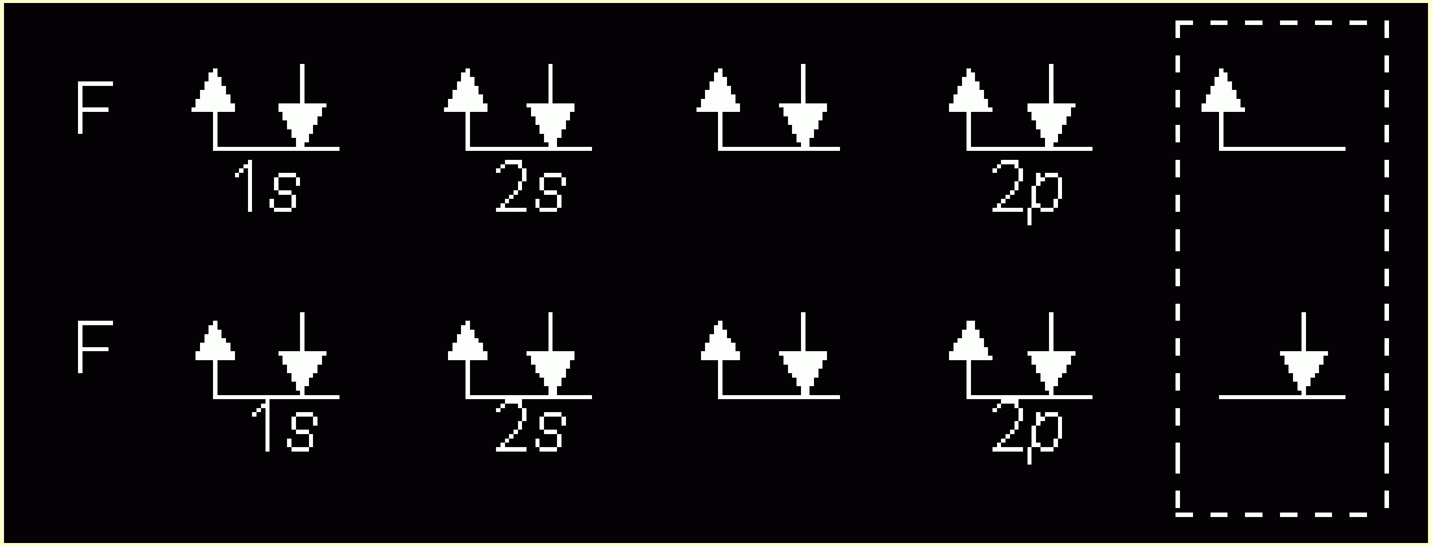




The Octet Rule – Covalent Compounds

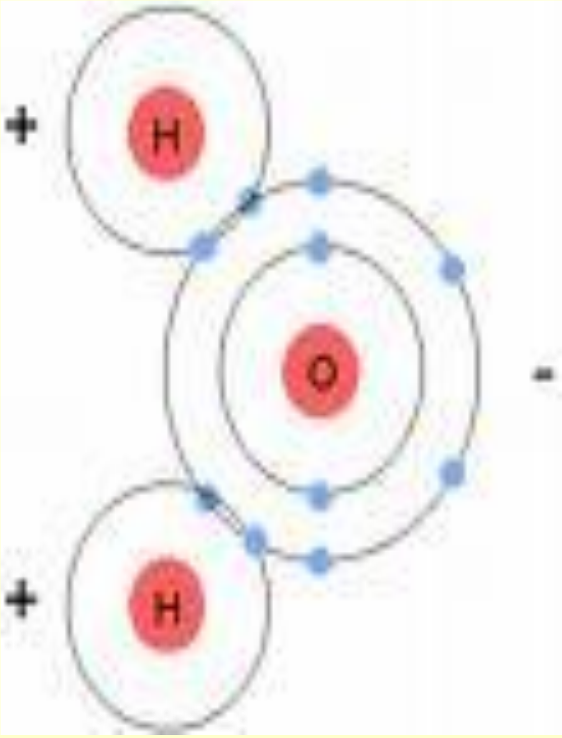
Covalent compounds tend to form so that each atom, by <u>sharing</u> electrons, has an octet of electrons in its highest occupied energy level.

Diatomic Fluorine



Covalent Bonds- force that holds two atoms together with shared electrons- most common bond

- Attraction of the positively charge nuclei to the shared negatively charged electrons



•Can share more than one pair of e^-

•Covalent compounds tend to form so that each atom, by <u>sharing</u> electrons, has an octet of electrons in its highest occupied energy level.

•Forms a molecule

Most Covalent Compounds are polar- unequal distribution of the electrons- one end positive and the other end negative

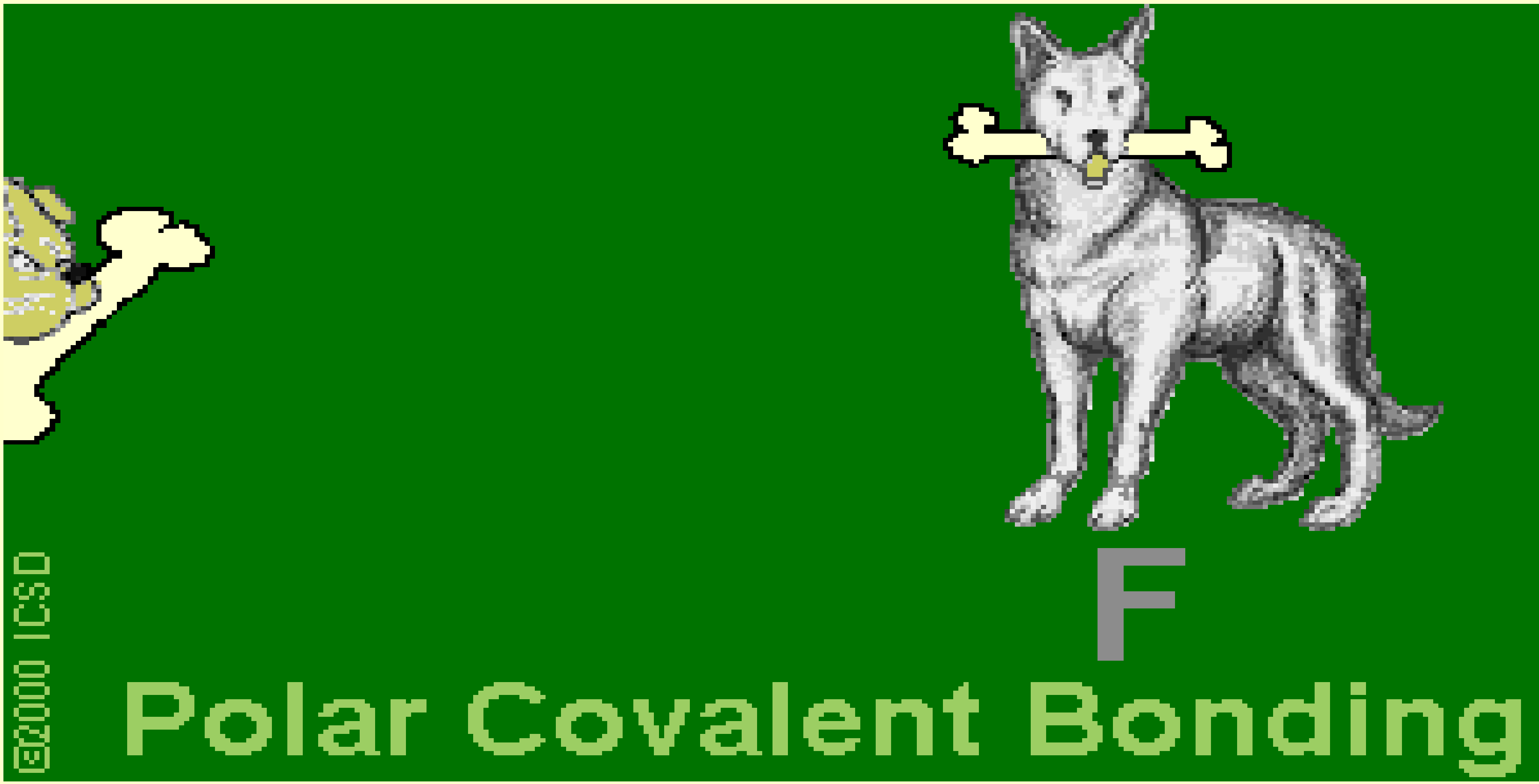
- Electrons will "spend" more time with the atom of highest electronegativity (attraction for electrons- the more non-metallic element) making that end of the molecule negative

Polar vs. Non-Polar

- **Non-polar covalent bonds have a small difference in electronegativites.**
  - *Equal* sharing of electron pairs.
    - Ex: H_2, N_2, etc.
- **Polar covalent bonds have a large difference in electronegativities.**
  - *Unequal* sharing of electron pairs.
    - *Creates dipoles!!!*
      - *Partial charges resulting from unequal sharing!*
    - *Ex: O–H in H_2O*

Polar Covalent Bonds:

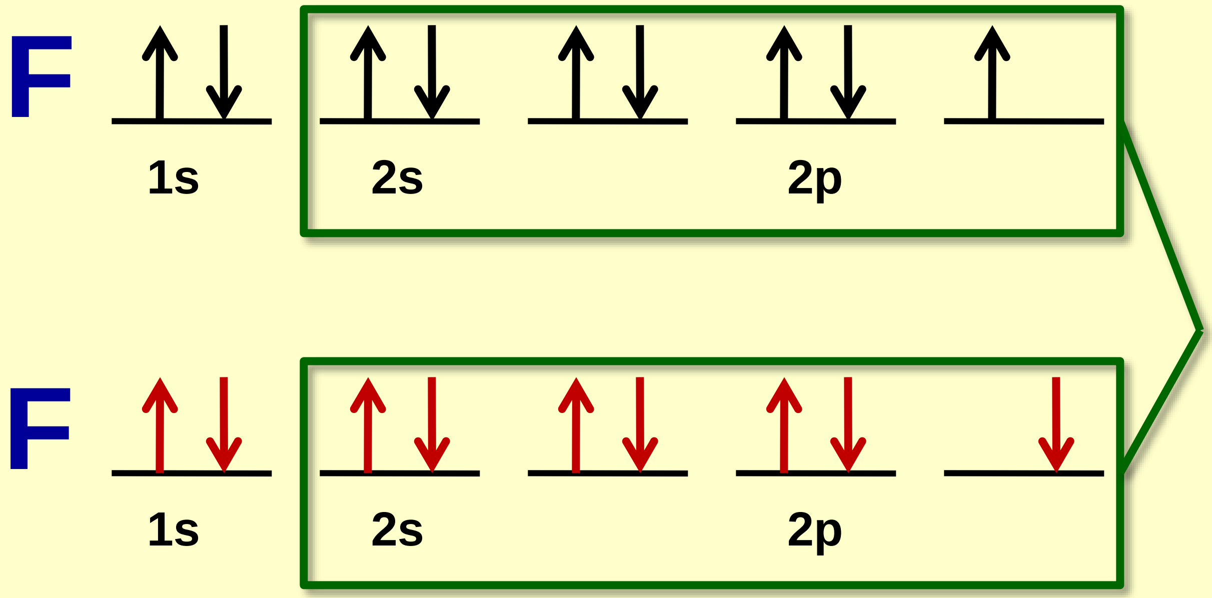
Unevenly matched, but willing to share.



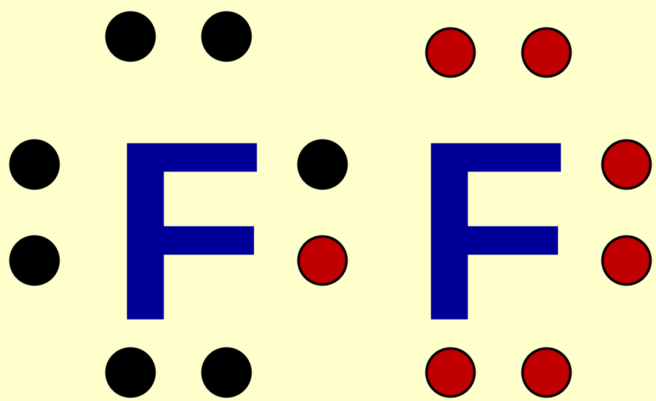
NON-POLAR COVALENT BONDS

Evenly Matched and willing to Share

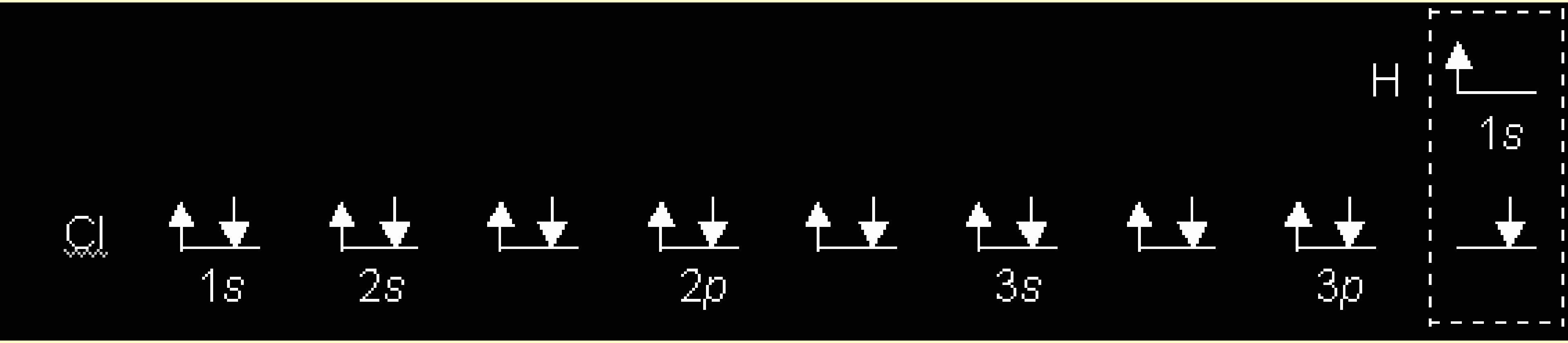
The Octet Rule:
The Diatomic Fluorine Molecule



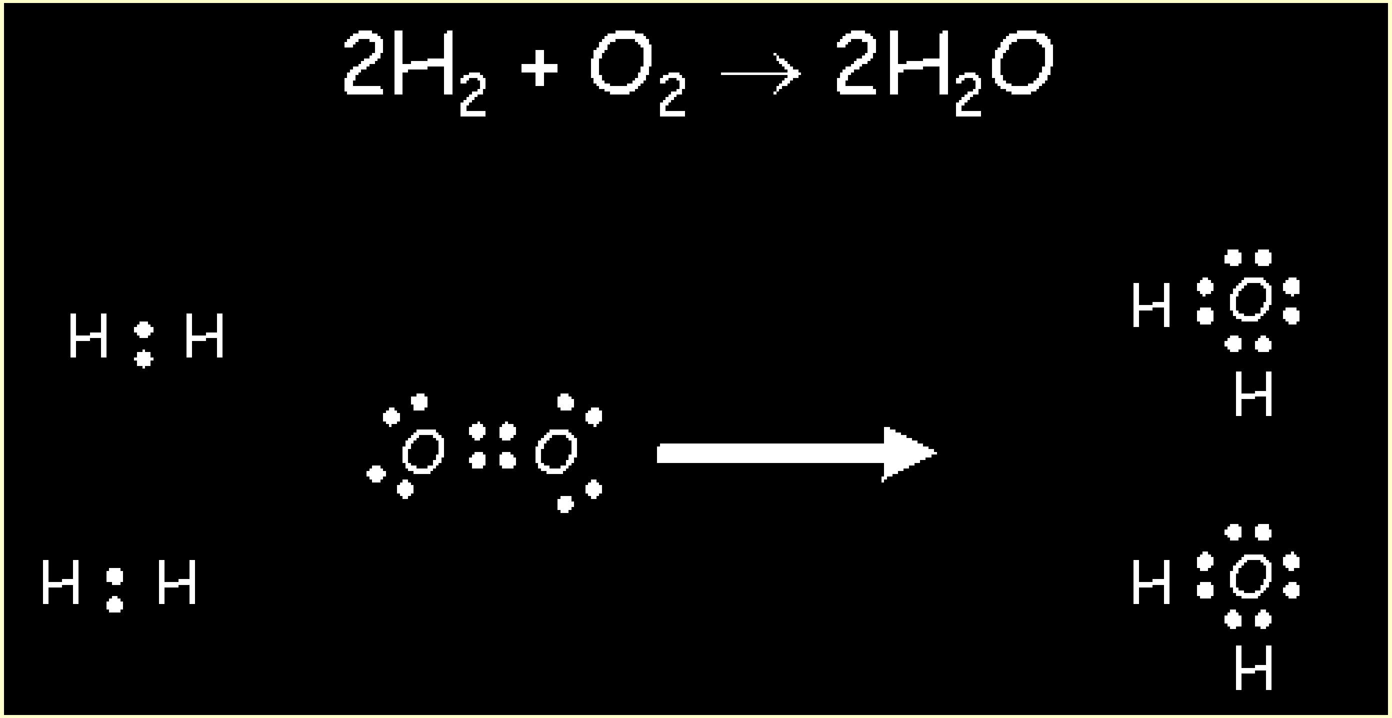
Each has ***seven*** valence electrons



Hydrogen Chloride by the Octet Rule



Formation of Water by the Octet Rule



Comments About the Octet Rule

- 2nd row elements C, N, O, F observe the octet rule.

- 2nd row elements B and Be often have fewer than 8 electrons around themselves - they are very reactive.

- 3rd row and heavier elements CAN exceed the octet rule using empty valence *d* orbitals.

- When writing Lewis structures, satisfy octets first, then place electrons around elements having available *d* orbitals.

Ionic Bonds are NOT necessarily stronger than Covalent Bonds !!!!!

How do we tell what type of bond will form?

Properties of Covalent Compounds

Phase:	Solid, liquid or gaseous
Melting point:	Varies depends on IPF
Boiling Point:	Varies
Electrical Conductivity:	Will not conduct under any conditions
Solubility in water:	Some are soluble but remain as a molecule
Volatility	Ranges depends on IPF

Electronegativity difference between the atoms determine the type of bond that will form between atoms (see table)

- If the difference is greater than 1.7 the bond will be mostly ionic in character

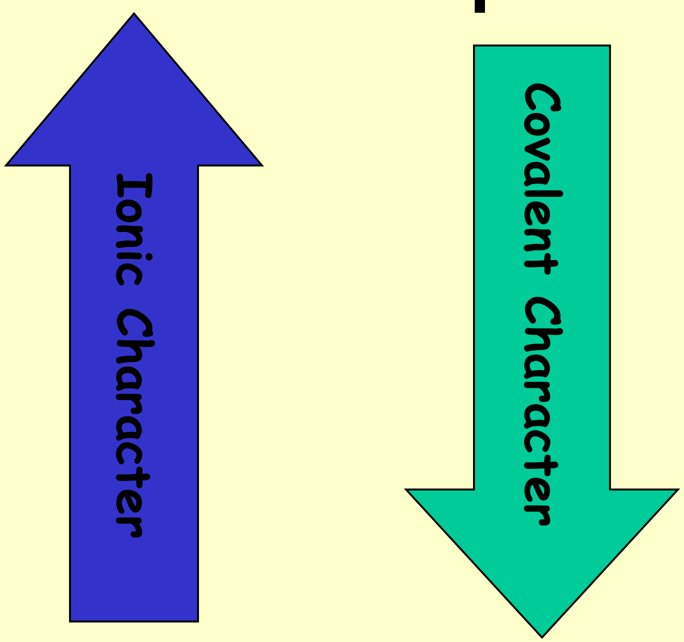
- If the difference is below 1.6 the bond will be mostly covalent in character:

Two types:

- Polar Covalent unequal sharing (1.6-0.4) &
- Non Polar Covalent equal sharing (0-0.3)

Determining Bond Type

- Take the difference between Pauling electronegativity values and correspond to the following chart.



3.3

| Ionic

1.7

| Polar Covalent

0.3

| Non-polar Covalent

0.0

below 1.0

1.0–1.4

1.5–1.9

2.0–2.4

2.5–2.9

3.0–4.0

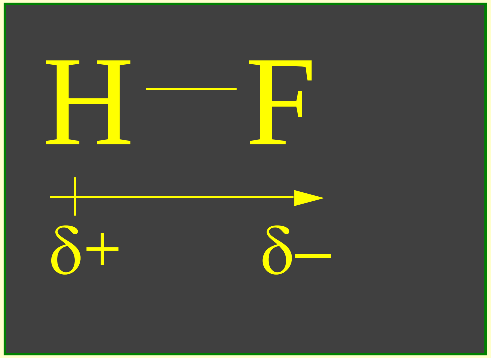
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
H 2.1																
Li 1.0	**Be** 1.5											**B** 2.0	**C** 2.5	**N** 3.0	**O** 3.5	**F** 4.0
Na 0.9	**Mg** 1.2											**Al** 1.5	**Si** 1.8	**P** 2.1	**S** 2.5	**Cl** 3.0
K 0.8	**Ca** 1.0	**Sc** 1.3	**Ti** 1.5	**V** 1.6	**Cr** 1.6	**Mn** 1.5	**Fe** 1.8	**Co** 1.8	**Ni** 1.8	**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 0.8	**Ba** 0.9	**La*** 1.1	**Hf** 1.3	**Ta** 1.5	**W** 2.4	**Re** 1.9	**Os** 2.2	**Ir** 2.2	**Pt** 2.2	**Au** 2.4	**Hg** 1.9	**Tl** 1.8	**Pb** 1.8	**Bi** 1.9	**Po** 2.0	**At** 2.2
Fr 0.7	**Ra** 0.9	**Ac†** 1.1														

*Lanthanides: 1.1–1.3

†Actinides: 1.3–1.5

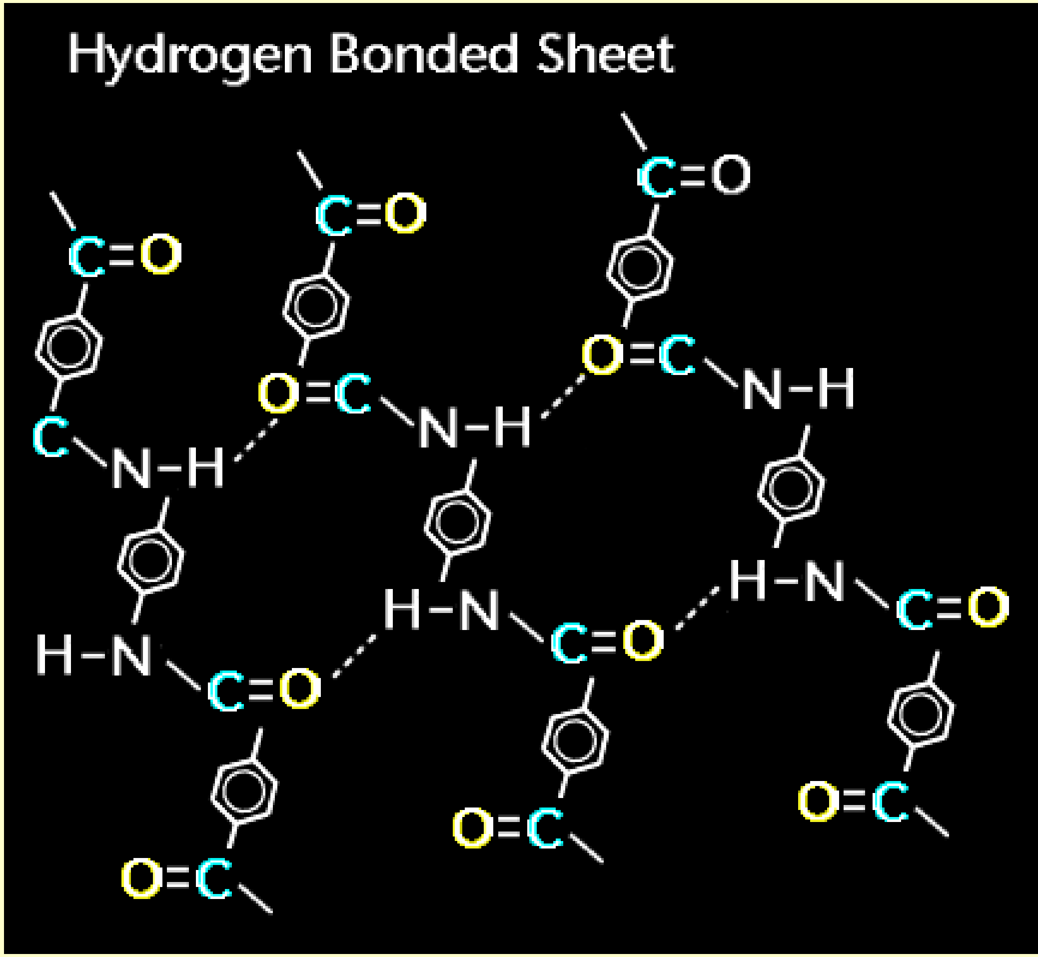
Polarity

A molecule, such as HF, that has a center of positive charge and a center of negative charge is said to be polar, or to have a dipole moment.



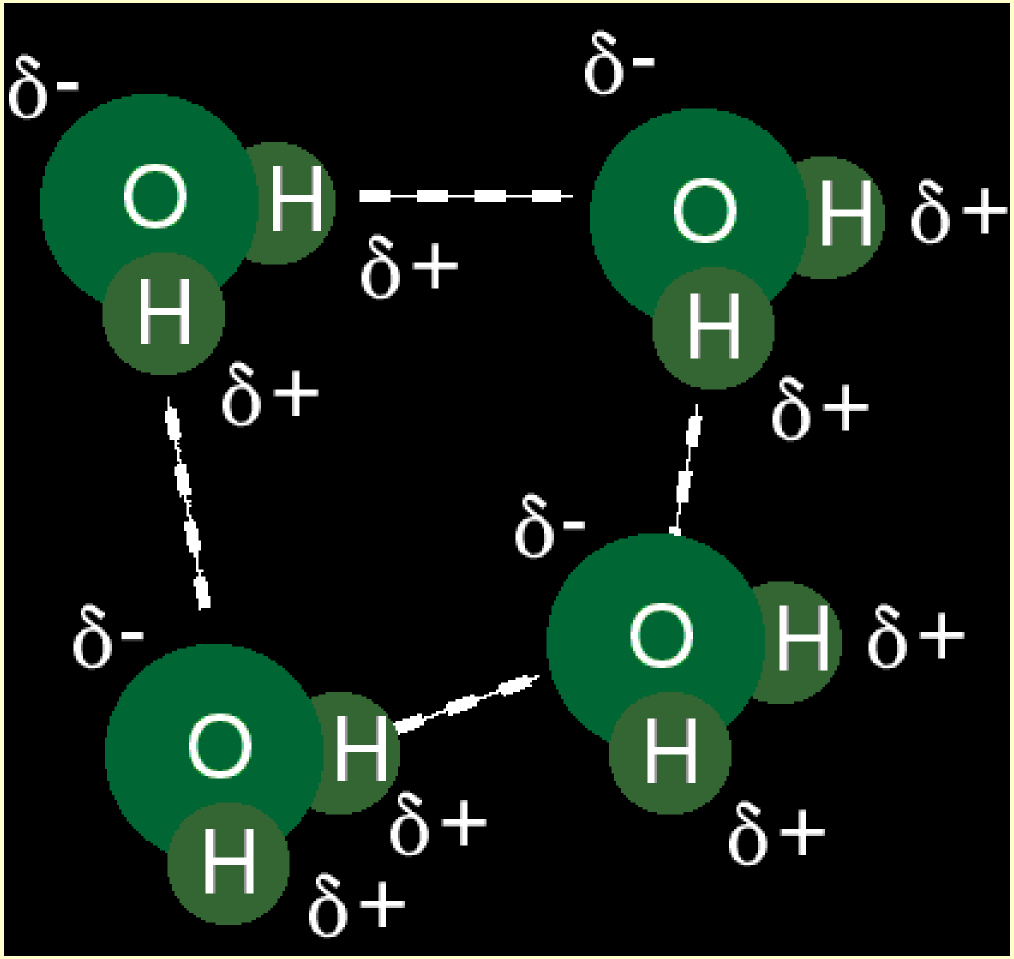
Hydrogen Bonding

Bonding between hydrogen and more electronegative neighboring atoms such as oxygen and nitrogen



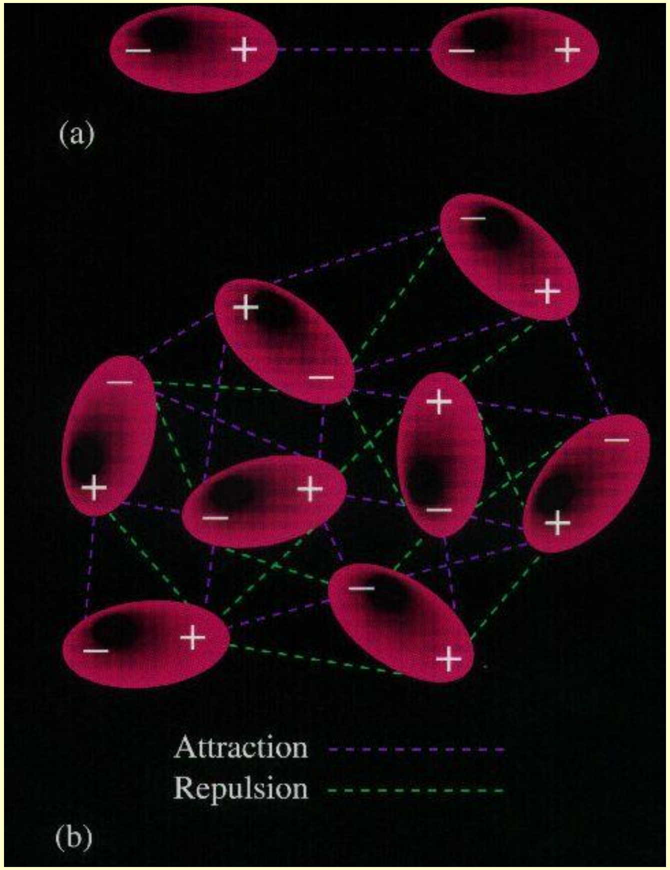
Hydrogen bonding in Kevlar, a strong polymer used in bullet-proof vests.

Hydrogen Bonding in Water



Dipole-Dipole Attractions

Attraction between oppositely charged regions of neighboring molecules.



London (Dispersion) Forces

- The weakest of intermolecular forces, these forces are proportional to the mass of the molecule
- These are the only forces of attraction between completely nonpolar molecules
  - Large nonpolar molecules may have substantial dispersion forces, resulting in relatively high boiling points
  - Small nonpolar molecules have weak dispersion forces and exist almost exclusively as gases

Relative magnitudes of forces

The types of bonding forces vary in their strength as measured by average bond energy.

Strongest

Covalent bonds (400 kcal)

Hydrogen bonding (12-16 kcal)

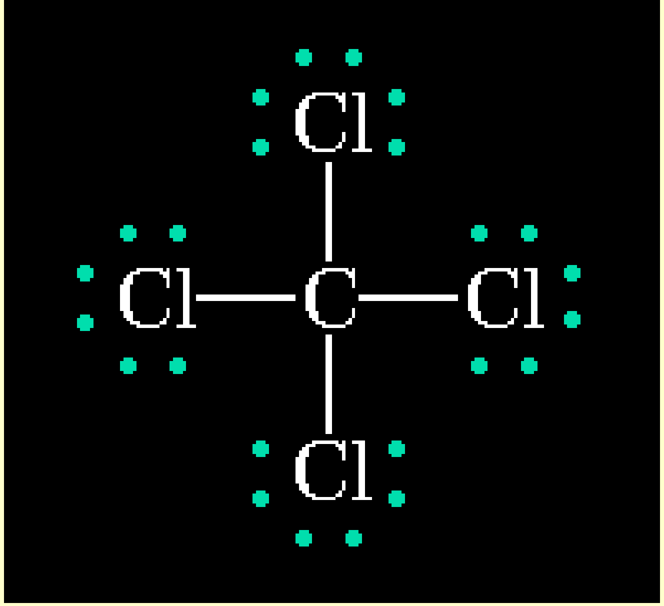
Dipole-dipole interactions (2-0.5 kcal)

London forces (less than 1 kcal)

Weakest

In A Glance:	Ionic	Covalent
Phase:	Crystalline solids	Solid, Liquid, or Gas
Force of Attraction between particles	High	Ranges
Melting point:	Generally high	Lower than Ionic
Boiling Point:	Generally high	Lower than Ionic
Conductivity:	Excellent conductors, molten and aqueous	**NEVER!!!**
Solubility water:	Quite Soluble	Ranges- Some are others aren't
Volatility	Low	Ranges

Lewis Structures



- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.

Completing a Lewis Structure –CH_3Cl

- Make carbon the central atom
- Join peripheral atoms to the central atom with electron pairs.
- Add up available valence electrons:

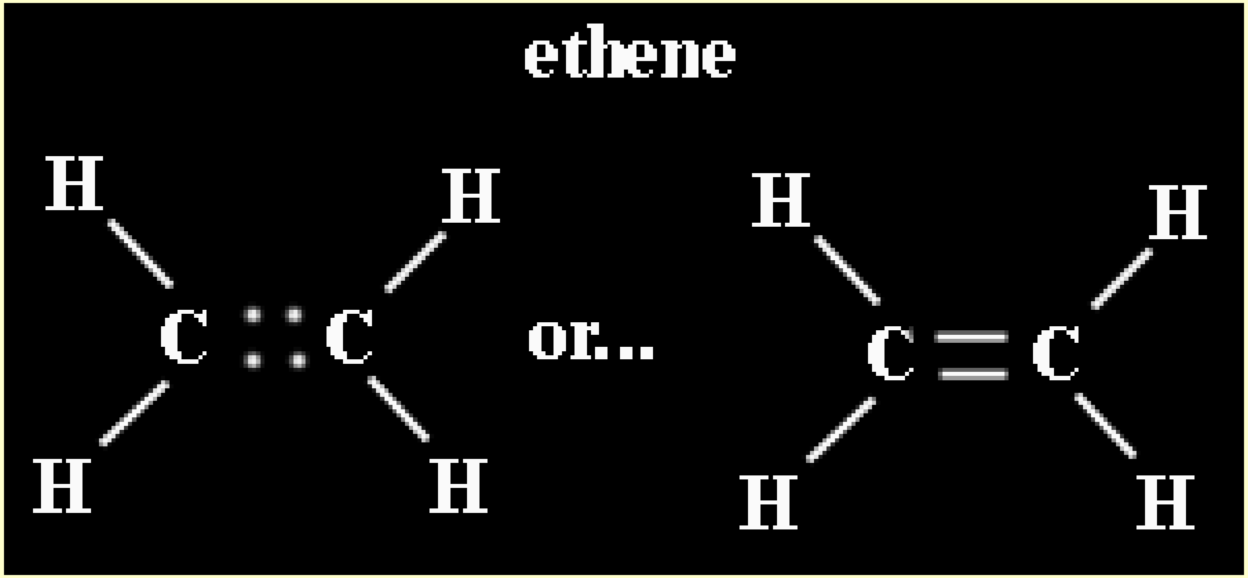
C = 4, H = (3)(1), Cl = 7   Total = 14

- Complete octets on atoms other than hydrogen with remaining electrons

H
··
H : C : Cl :
··
H

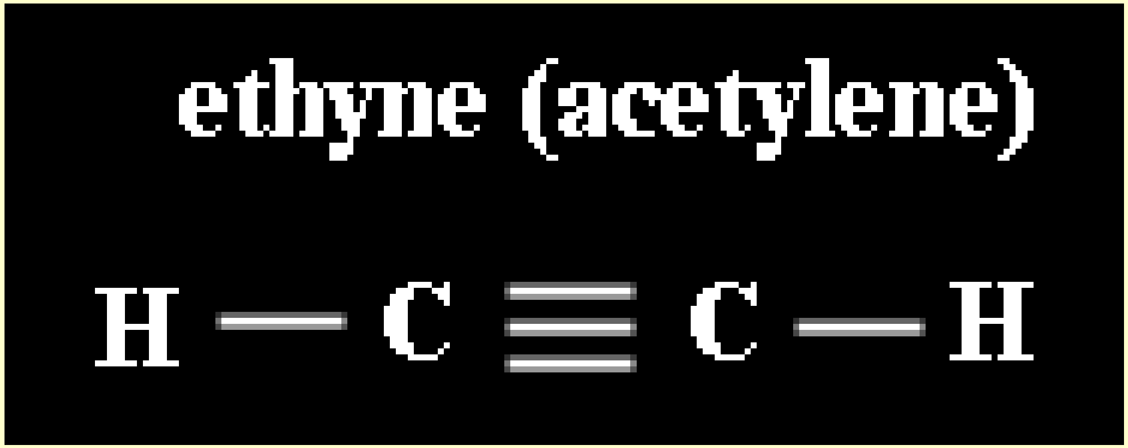
Is this molecule polar?

Multiple Covalent Bonds: Double bonds



Two pairs of shared electrons

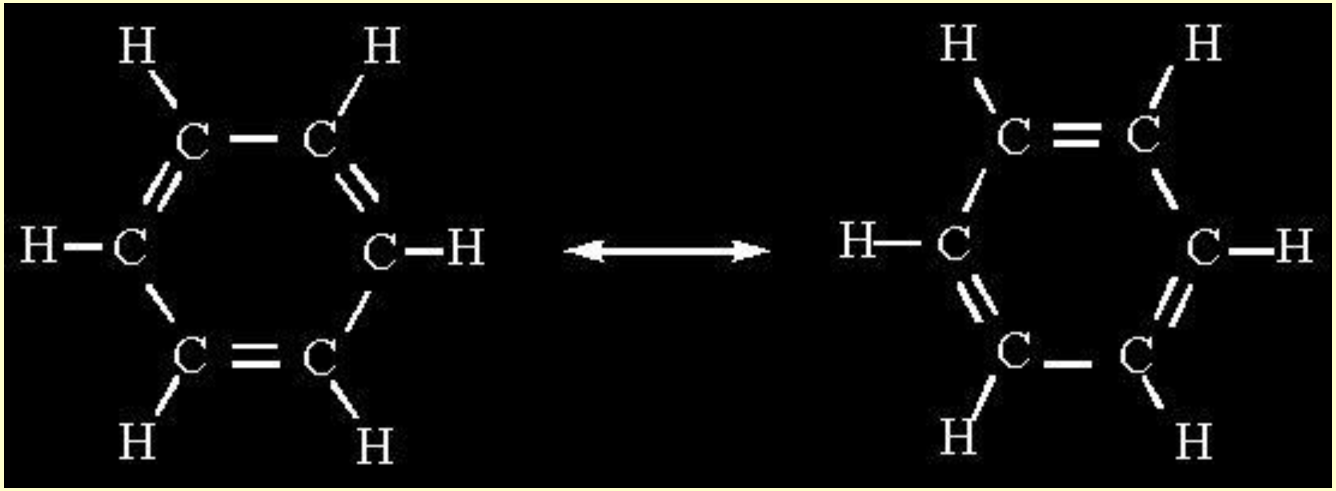
Multiple Covalent Bonds:
Triple bonds



Three pairs of shared electrons

Resonance

Occurs when more than one valid Lewis structure can be written for a particular molecule.



- These are resonance structures.

  The actual structure is an average of the resonance structures.

H_2S

CF_4

SiO_2

P_2

What is the correlation between bond length and bond energy (energy required to break the bond)?

Bond Length and Bond Energy

Bond	*Length (pm)*	*Energy (kJ/mol)*
C - C	154	346
C=C	134	612
C≡C	120	835
C - N	147	305
C=N	132	615
C≡N	116	887
C - O	143	358
C=O	120	799
C≡O	113	1072
N - N	145	180
N=N	125	418
N≡N	110	942

Models

Models are attempts to explain how nature operates on the microscopic level based on experiences in the macroscopic world.

Models can be physical as with this DNA model

Models can be mathematical

Models can be theoretical or philosophical

Fundamental Properties of Models

- A model does not equal reality.
- Models are oversimplifications, and are therefore often wrong.
- Models become more complicated as they age.
- We must understand the underlying assumptions in a model so that we don't misuse it.

VSEPR Model

(Valence Shell Electron Pair Repulsion)

- VSEPR Theory is based on the idea that groups of electrons repel each other as far away as possible within a molecule.
- The structure (shape) around a given atom is determined *principally* by minimizing electron pair repulsions.

(negative-negative repulsions)

Predicting a VSEPR Structure

1. Draw Lewis structure.
2. Put pairs as far apart as possible
3. Determine positions of atoms from the way electron pairs are shared.
4. Determine the name of molecular structure from positions of the atoms.

VSPER MODELS TO KNOW

- 2 Substituents ➔ Linear (180^0 angle)
- 2 Subs +1 or 2 unshared pair → Bent
- 3 Subs ➔ Triangular planar (120^0 angle)
- 3 Subs + 1 unshared pair → Trigonal Pyramidal (<120)
- 4 Substituents ➔ Tetrahedral (109.5^o angle)

Is My Molecule Polar?

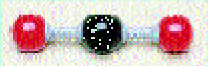
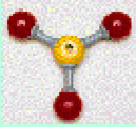
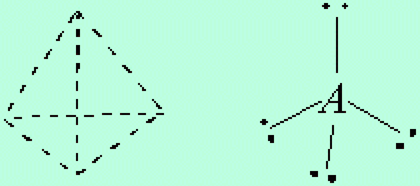
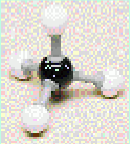
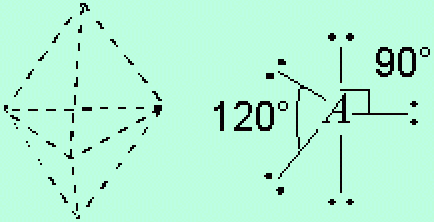
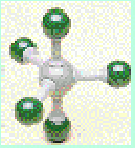
1 atom attached Linear: NonPolar if same atoms
Polar if different atoms

2 atoms attached Linear: NonPolar if same atoms
Polar if different atoms
Bent: Polar due to unbonded electrons

3 atoms attached Trigonal planer: NonPolar if same atoms
Polar if different
Trigonal Pyramidal: Polar due to unbonded electrons

4 atoms attached Tetrahedral: NonPolar if same atoms
Polar if different atoms

Table 8.6 Arrangements of Electron Pairs Around an Atom Yielding Minimum Repulsion

Number of Electron Pairs		Arrangement of Electron Pairs	Example
2	Linear		
3	Trigonal planar		
4	Tetrahedral		
5	Trigonal bipyramidal		
6	Octahedral