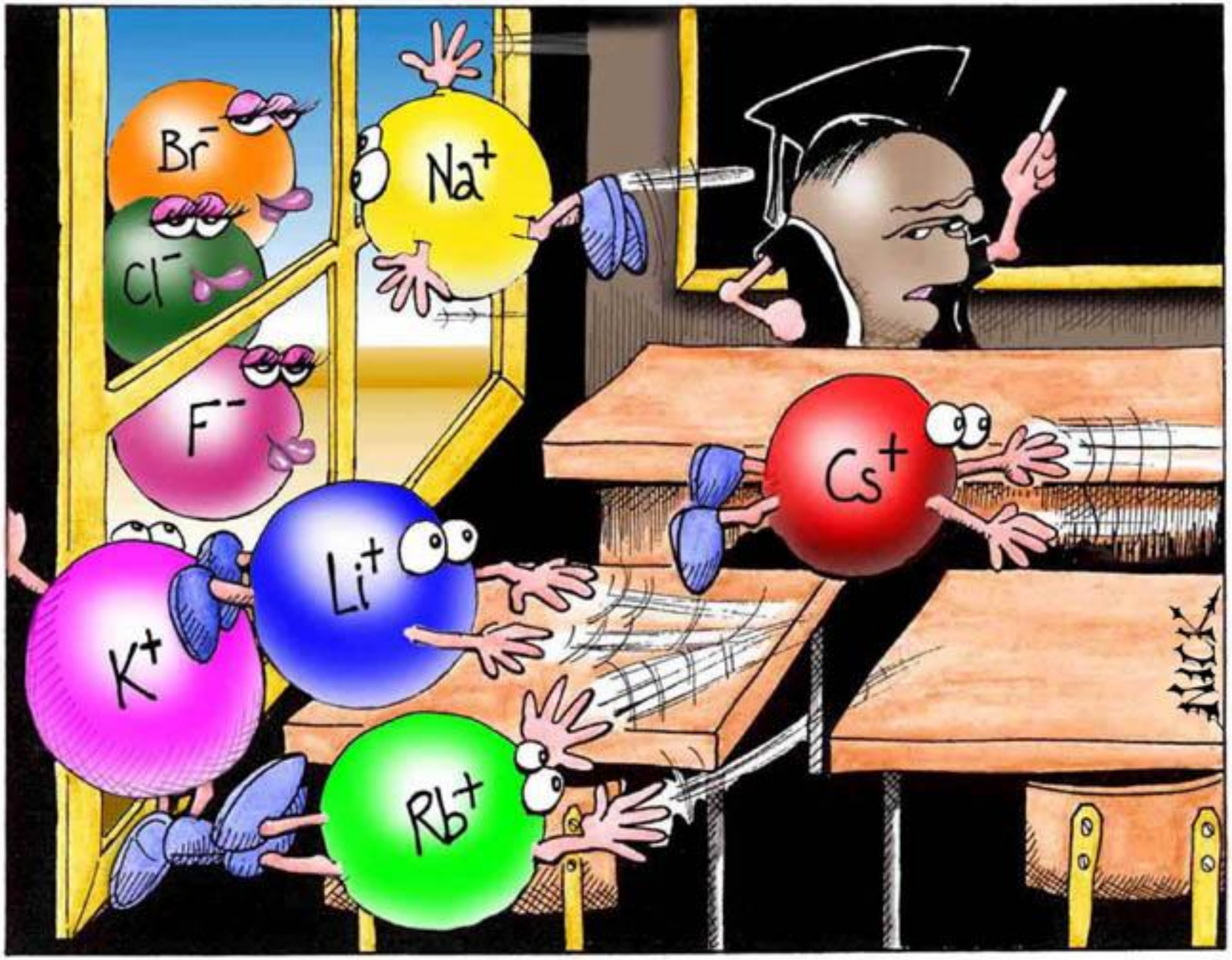
Chemical Bonding and Molecular Structure



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

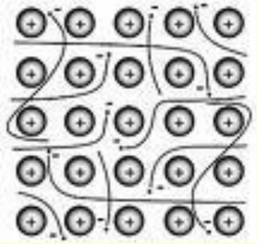
Cartoon courtesy of NearingZero.net

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

Metallic Bonding

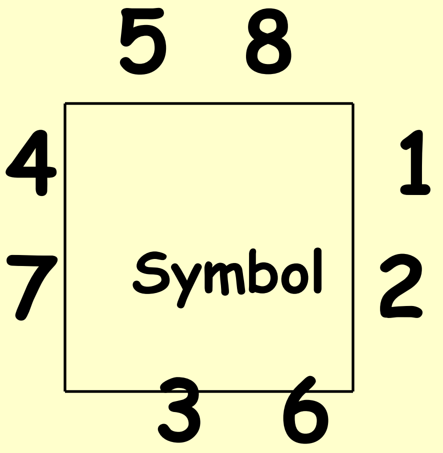


- The chemical bonding that results from the attraction between protons in metal nuclei and the surrounding sea of electrons (Copper, iron, aluminum)

- 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



5 8

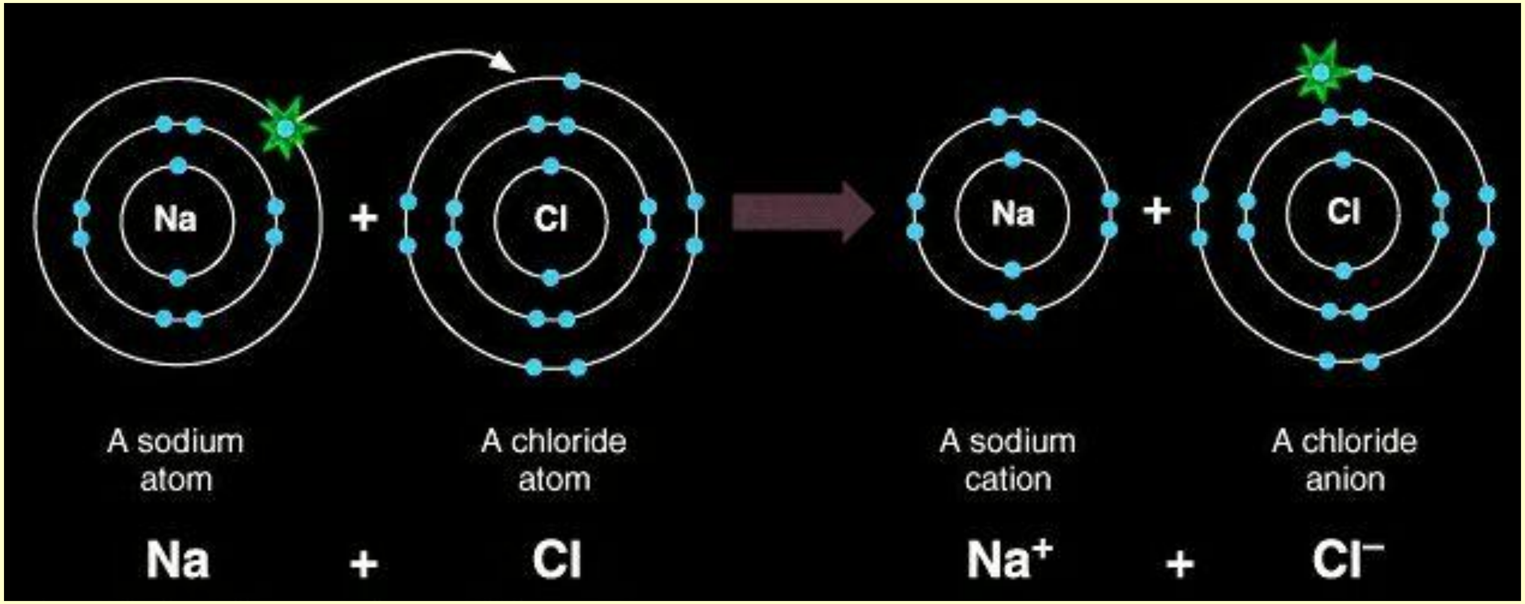
4 1

7 Symbol 2

3 6

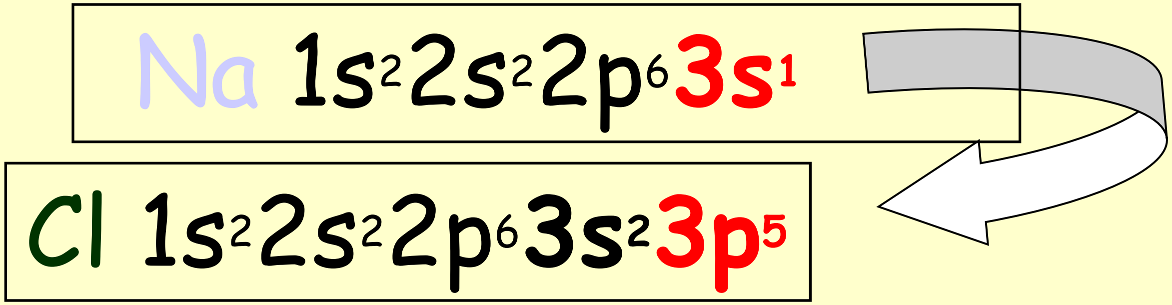
The **Octet** Rule – Ionic Compounds

Ionic compounds tend to form so that each atom, by gaining or losing 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 octet**:

Cation→ Na^+ $1s^2 \boxed{2s^2 2p^6}$

Anion→Cl^- $1s^2 2s^2 2p^6 \boxed{\mathbf{3s^2 3p^6}}$

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

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

+

→

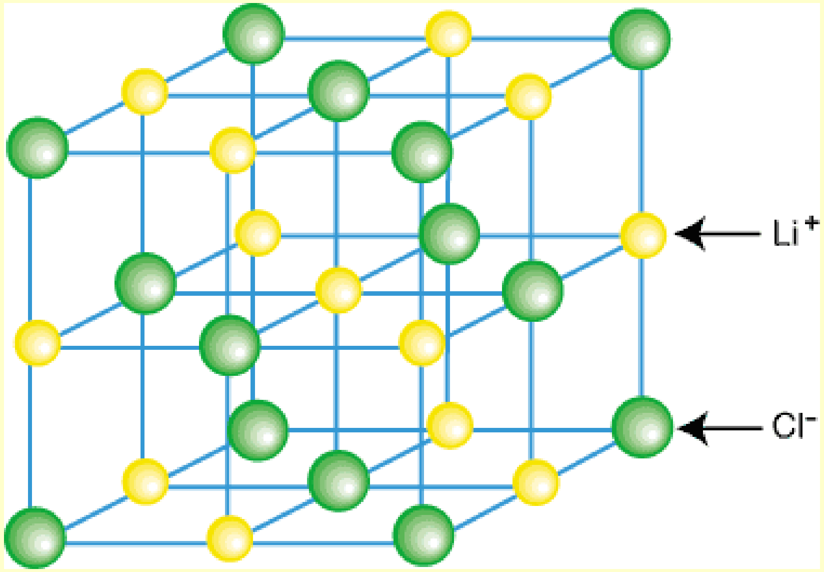
Silver-colored Metal

Poisonous Green Gas

White Crystal

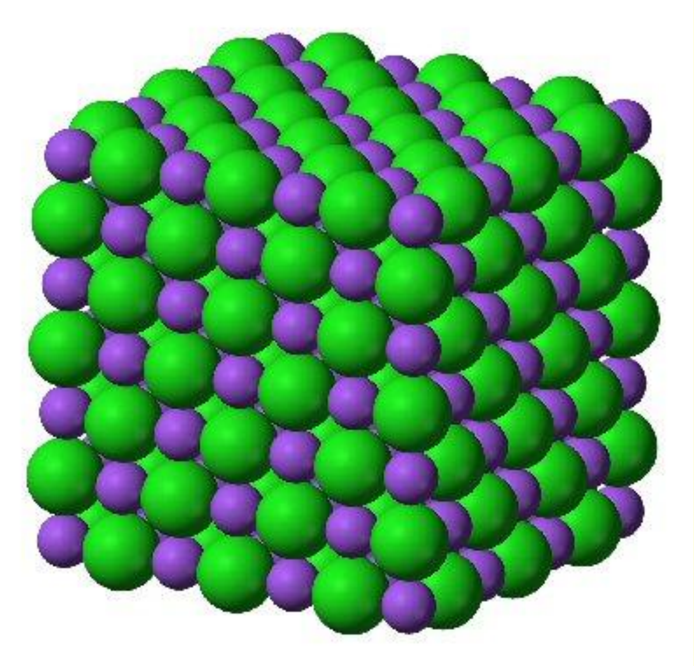
Representation of Components in an Ionic Solid

Lattice: A 3-dimensional system of points designating the centers of components (atoms, ions, or molecules) that make up the substance **alternating positive and negative ions.**



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

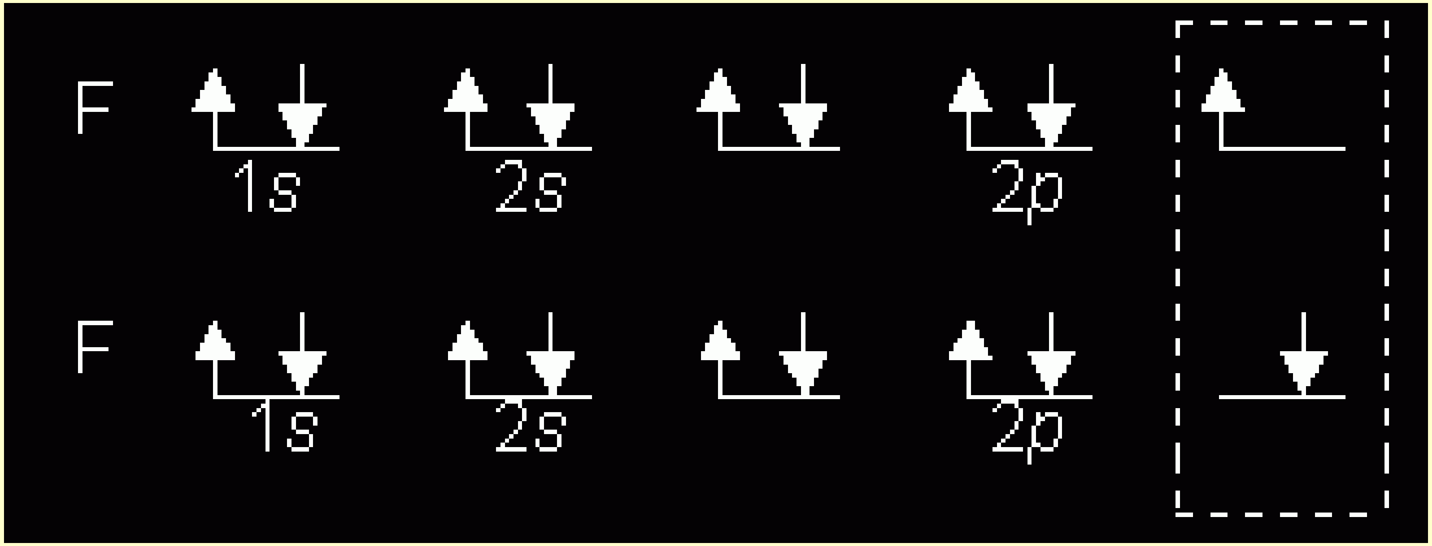
Properties of Ionic Compounds

IPF	HIGH particles are "locked" together
State	Crystalline solids
Melting point:	Generally high
Boiling Point:	Generally high
Electrical Conductivity:	Excellent conductors, molten and aqueous
Solubility in water:	Generally Quite Soluble
Volatility (ability to evaporate)	Low

The Octet Rule – Covalent Compounds

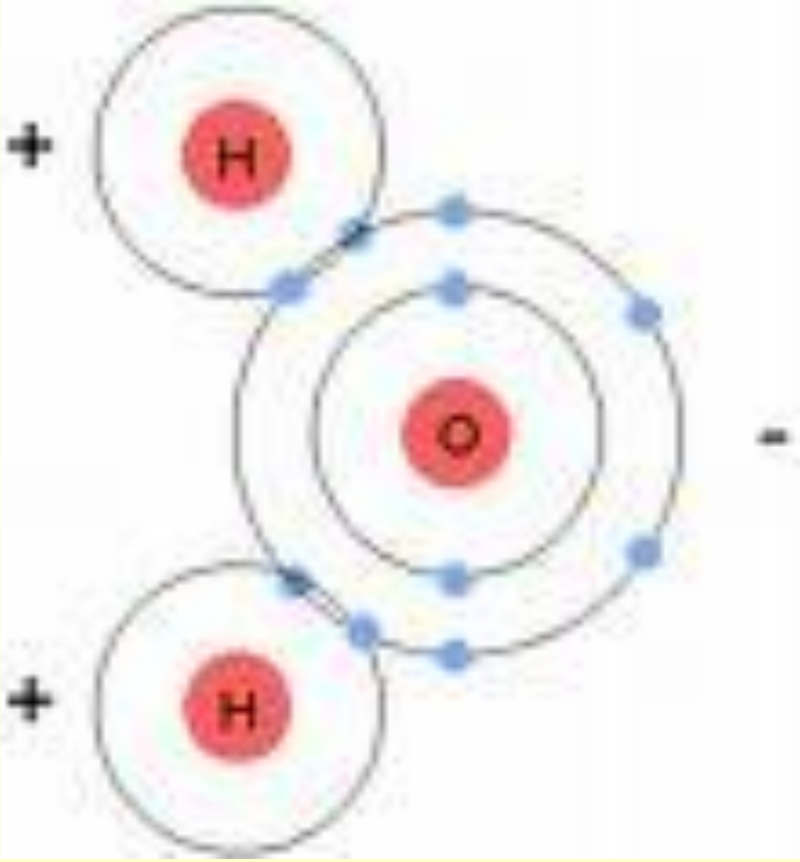
Covalent compounds tend to form so that each atom, by sharing electrons, has an octet of electrons in its highest occupied energy level. The P orbitals overlap and electrons are shared

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

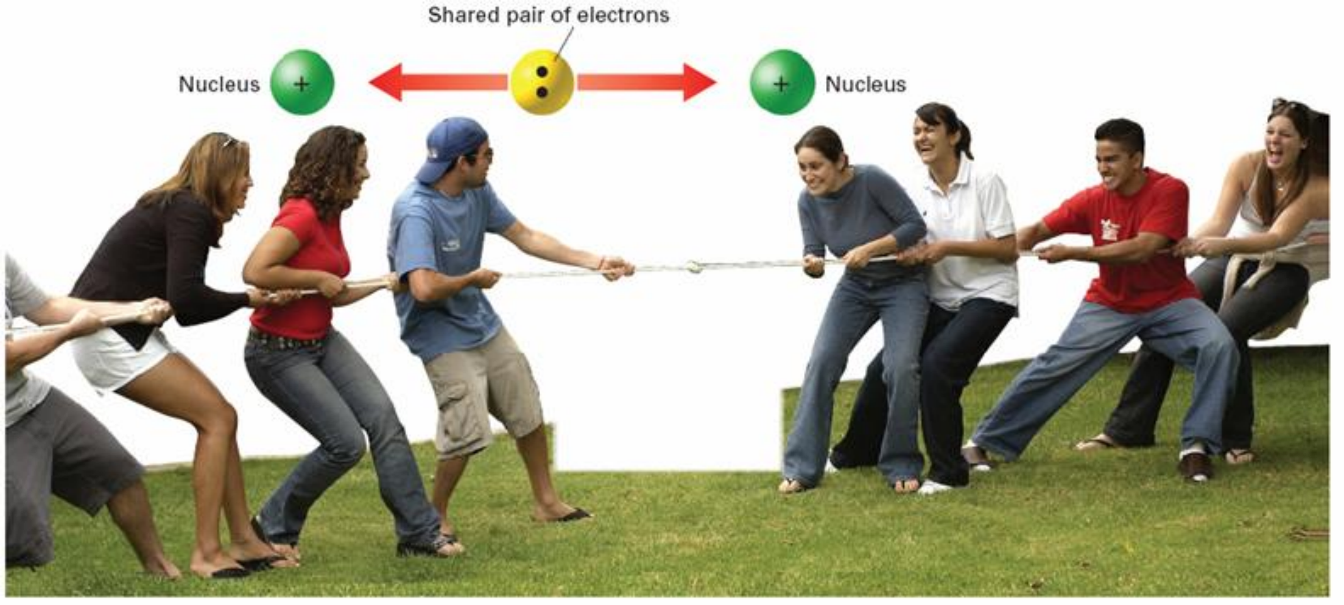


•Can share more than one pair of e$^-$

•Forms a molecule

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

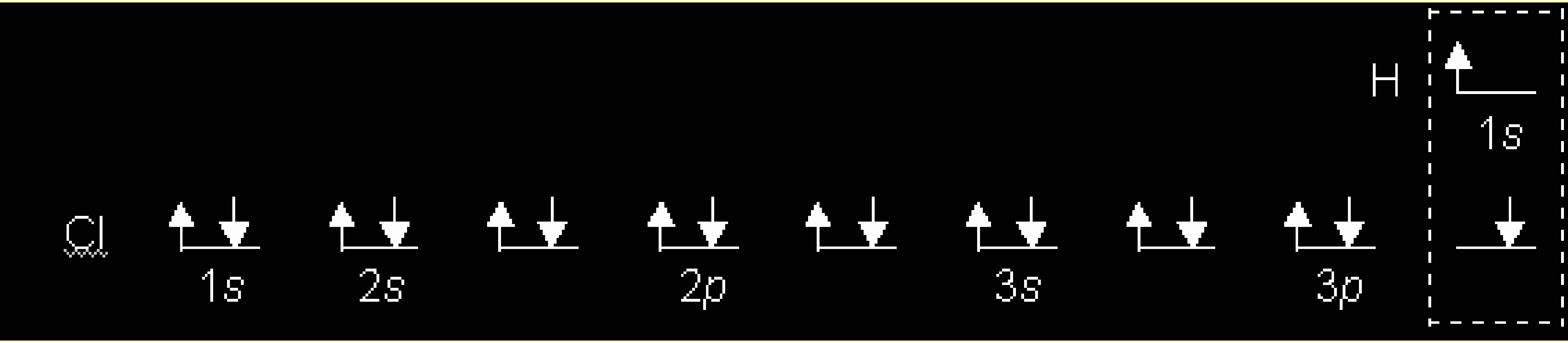
- Electrons will "spend" more time with the atom of highest electronegativity (attraction for electrons- the more non-metallic element) making that end of the molecule negative



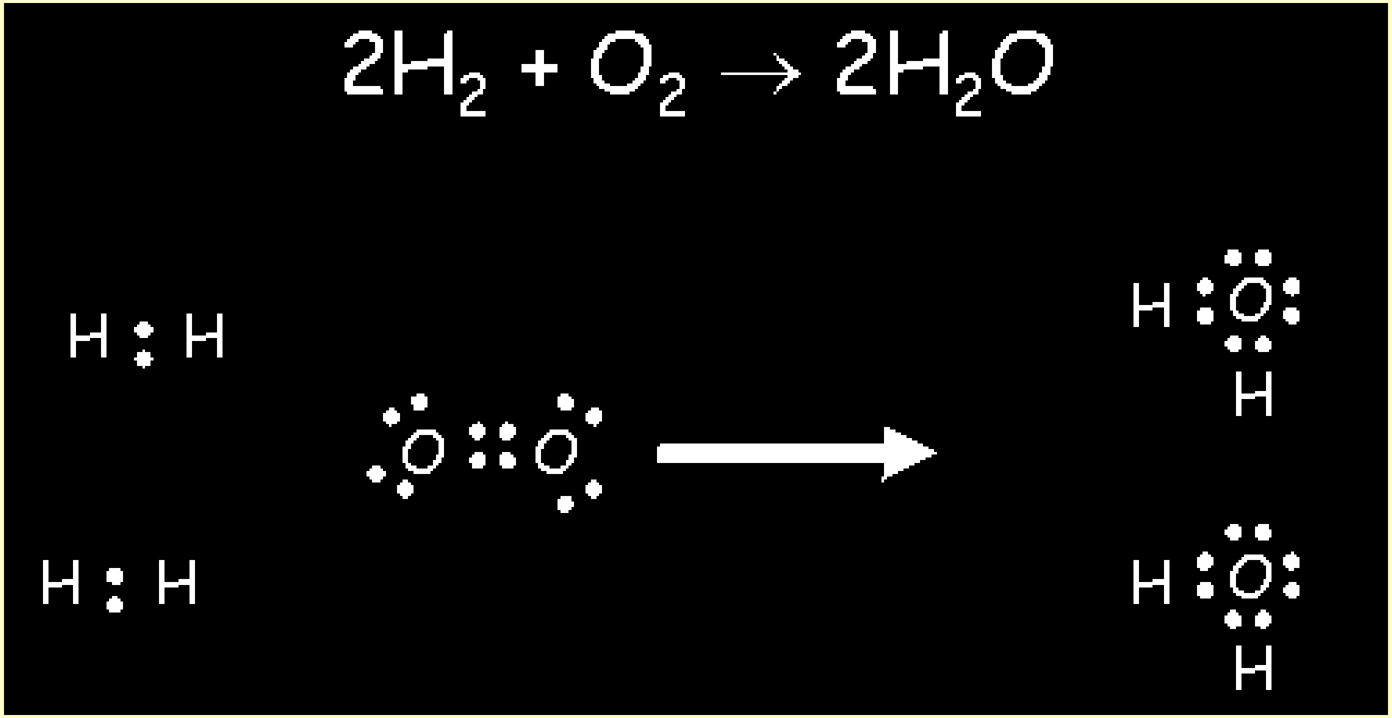
Hydrogen Chloride by the Octet Rule

Hydrogen's S orbital overlaps with Chlorine's P orbital

Hydrogen has satisfied the duet rule and chlorine has satisfied the octet rule



Formation of Water by the Octet Rule



$2H_2 + O_2 \rightarrow 2H_2O$

Comments About the Octet Rule

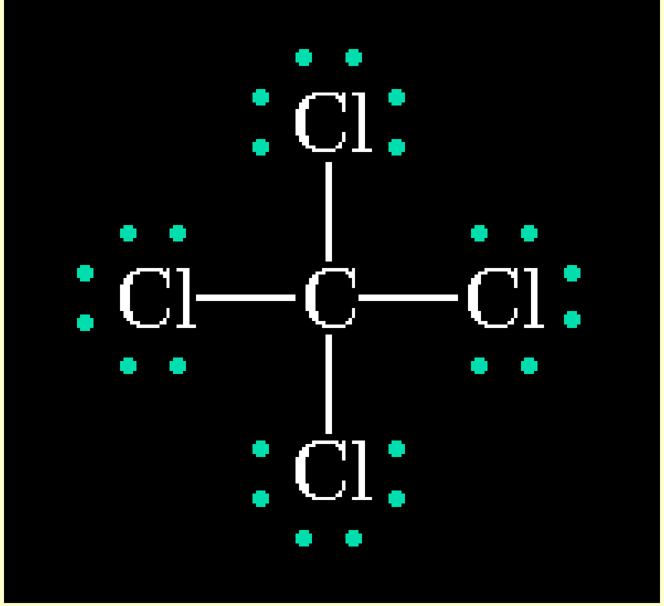
- 2nd row elements C, N, O, F observe the octet rule.

- 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.

Lewis Structures

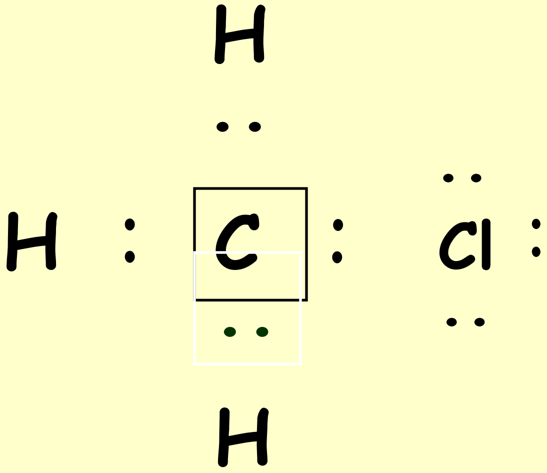


- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.

Completing a Lewis Structure -CH_3Cl

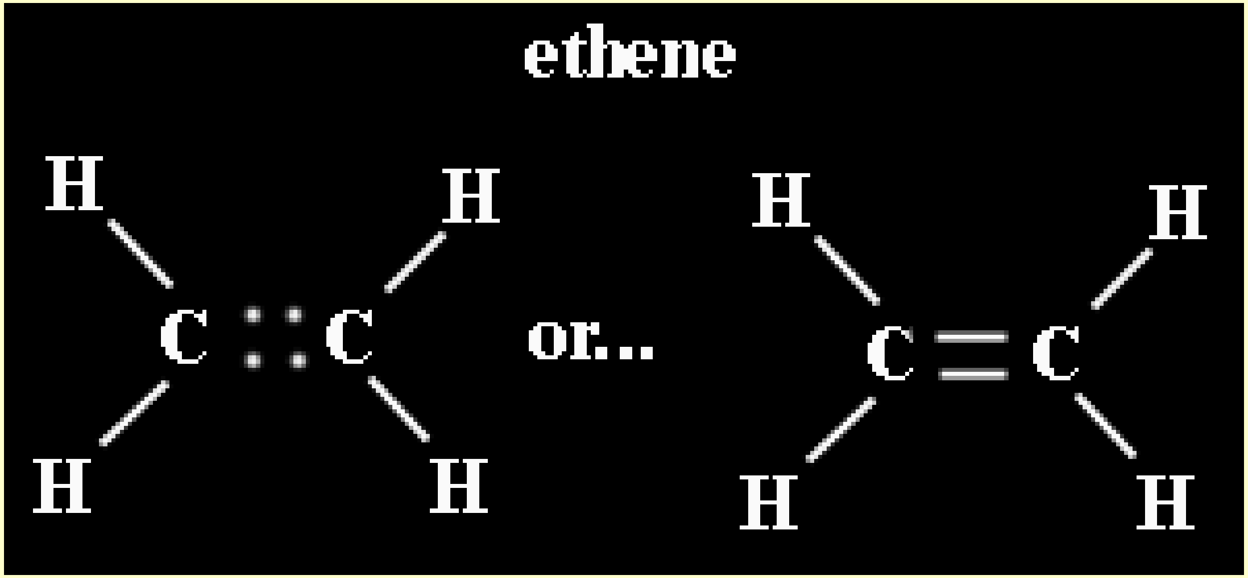
- Make carbon the central atom
- Join peripheral atoms to the central atom with electron pairs.
- Complete octets on atoms other than hydrogen with remaining electrons

Is this molecule polar?



Multiple Covalent Bonds:

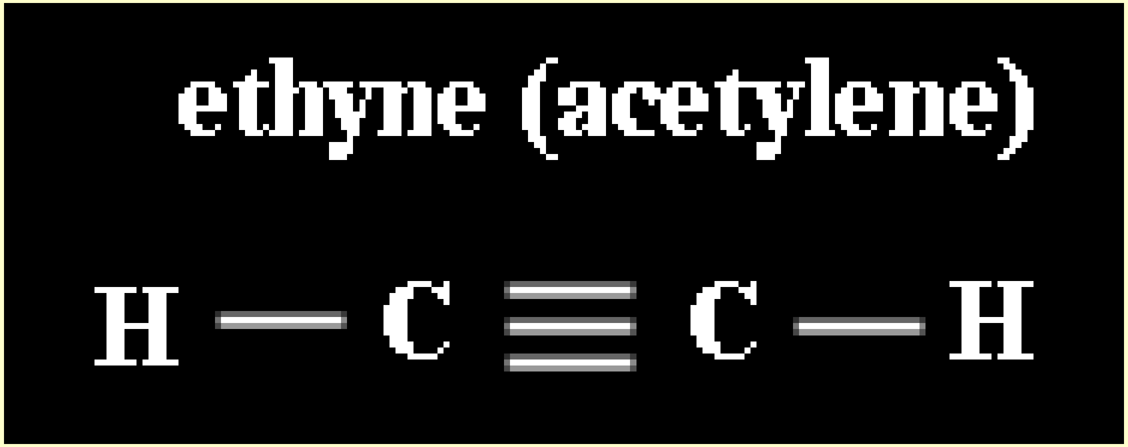
Double bonds



Two pairs of shared electrons

Multiple Covalent Bonds:

Triple bonds



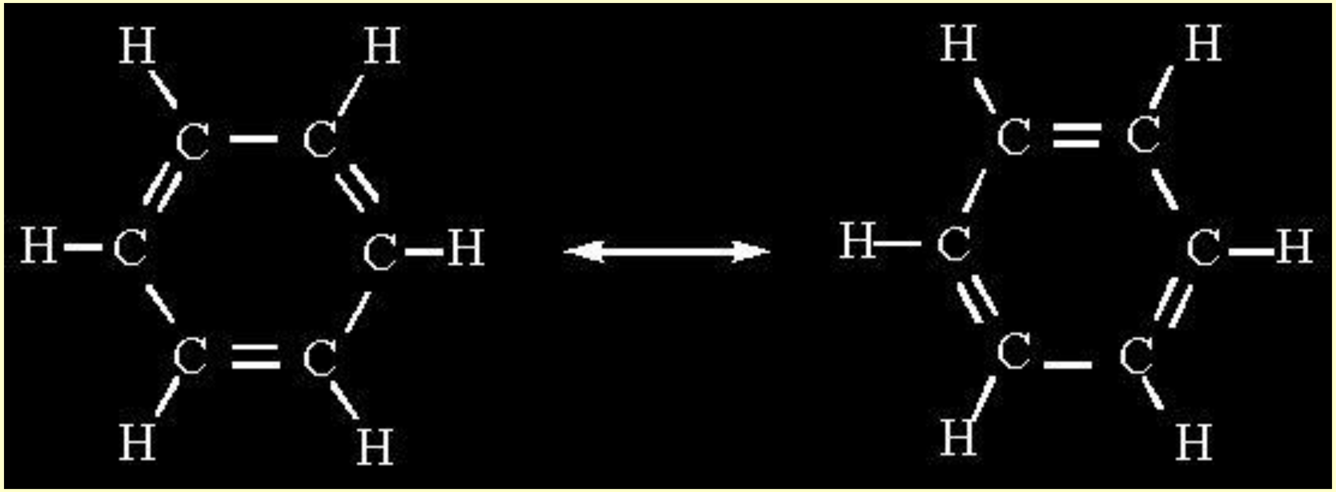
ethyne (acetylene)

$H - C \equiv C - H$

Three pairs of shared electrons

Resonance

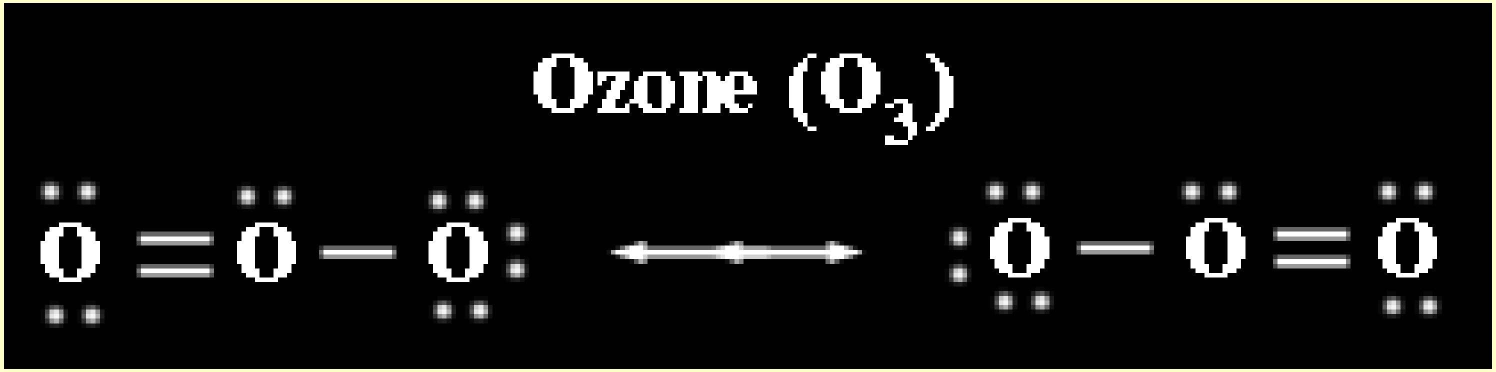
Occurs when more than one valid Lewis structure can be written for a particular molecule.



- These are resonance structures.

  The actual structure is an average of the resonance structures.

Resonance in Ozone



Neither structure is correct. The molecule exists somewhere in between and bond FLIPS

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

Properties of Covalent Compounds

IMF:	Varies
Phase:	Solid, liquid or gaseous
Melting point:	Varies depends on IMF
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 IMF

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 dep on IMF
Volatility	Low	Ranges

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

Would be comparing apples and oranges!

Could look at bond length and lattice energy BUT NOT THE SAME-

Think about melting points…
Nitrogen- Strong Covalent bond- gas
Sodium Chloride- Strong Ionic Bond- Solid

Different forces account for the many differences in physical properties of compounds such as physical state, degree of volatility (ability to turn into a gas), solubility, melting point, and conductivity of covalent and ionic compounds.

Why is water a liquid at room temperature but carbon dioxide a gas?

How do we tell what type of bond will form

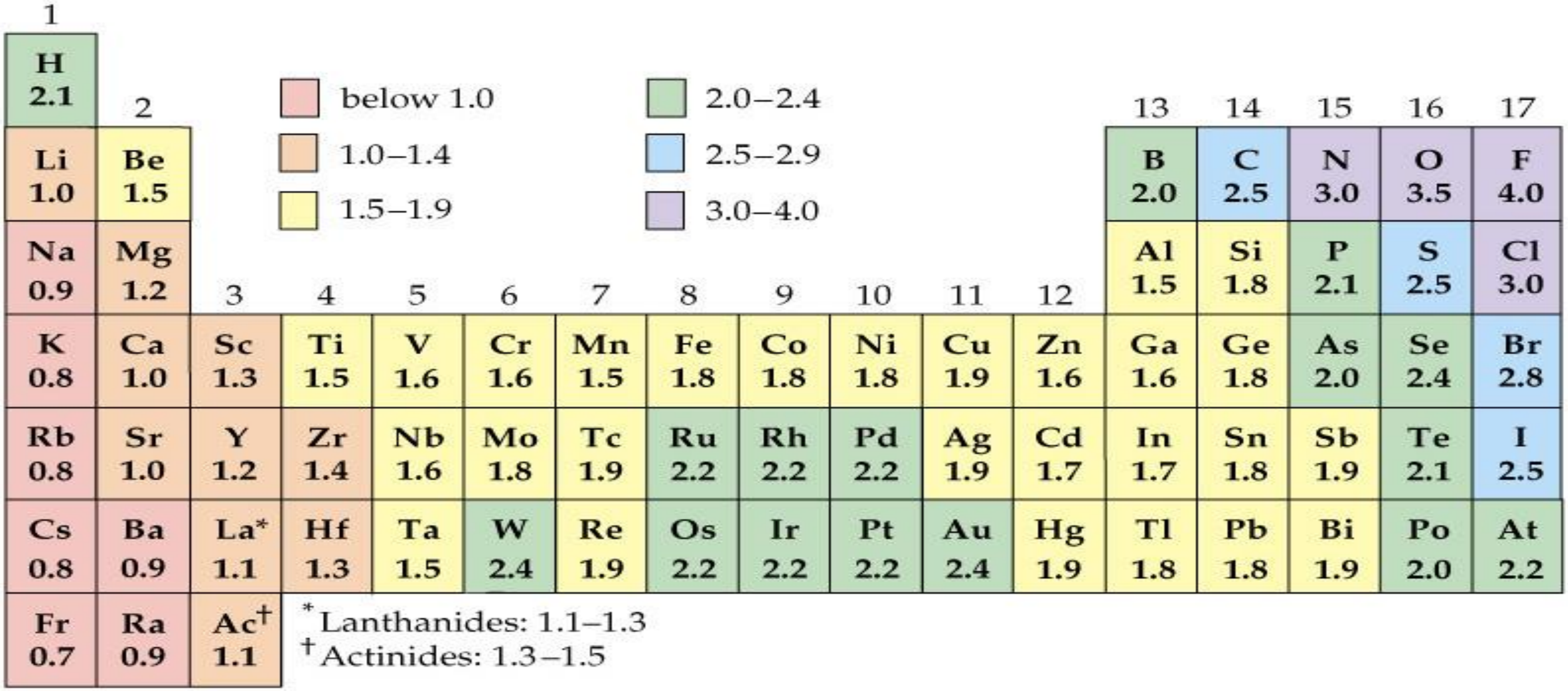
Electronegativity difference between the atoms determine the type of bond that will form between atoms (see table on next slide)

- 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)



🟥 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

Determine the Bond Character Between:

Lithium and Bromine

Sulfur and Selenium

Carbon and Oxygen

Carbon & Hydrogen can only form covalent bonds !

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)

The structure 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

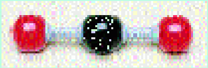
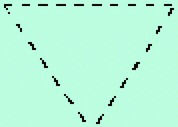
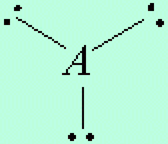
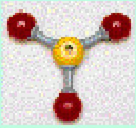
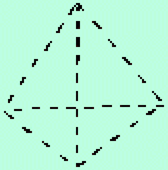
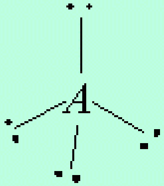
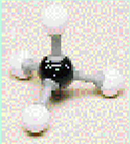
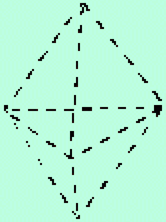
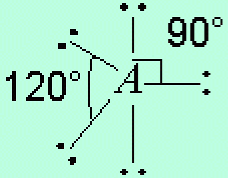
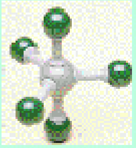
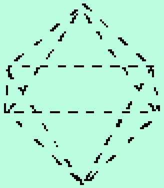
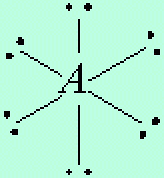
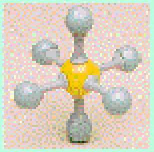
3. Determine positions of atoms from the way electron pairs are shared.

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)

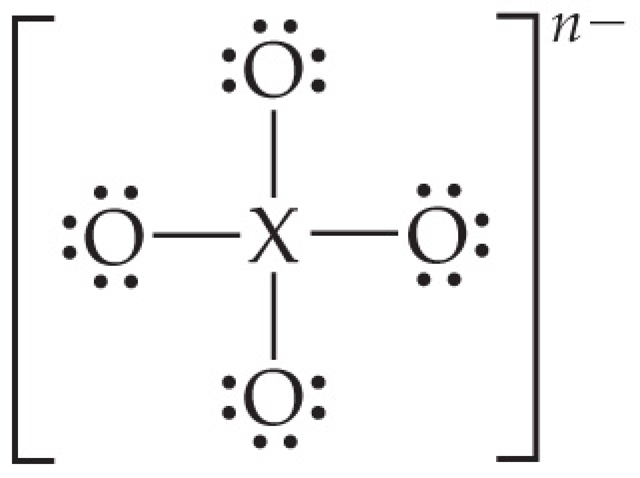
Table 8.6 Arrangements of Electron Pairs Around an Atom Yielding Minimum Repulsion

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

Polyatomic Ions-

group of covalently joined atoms that carry a charge AKA radical group

Negative Charge indicates more electrons are added to create the octet
Positive Charge indicates electrons removed to create the octet



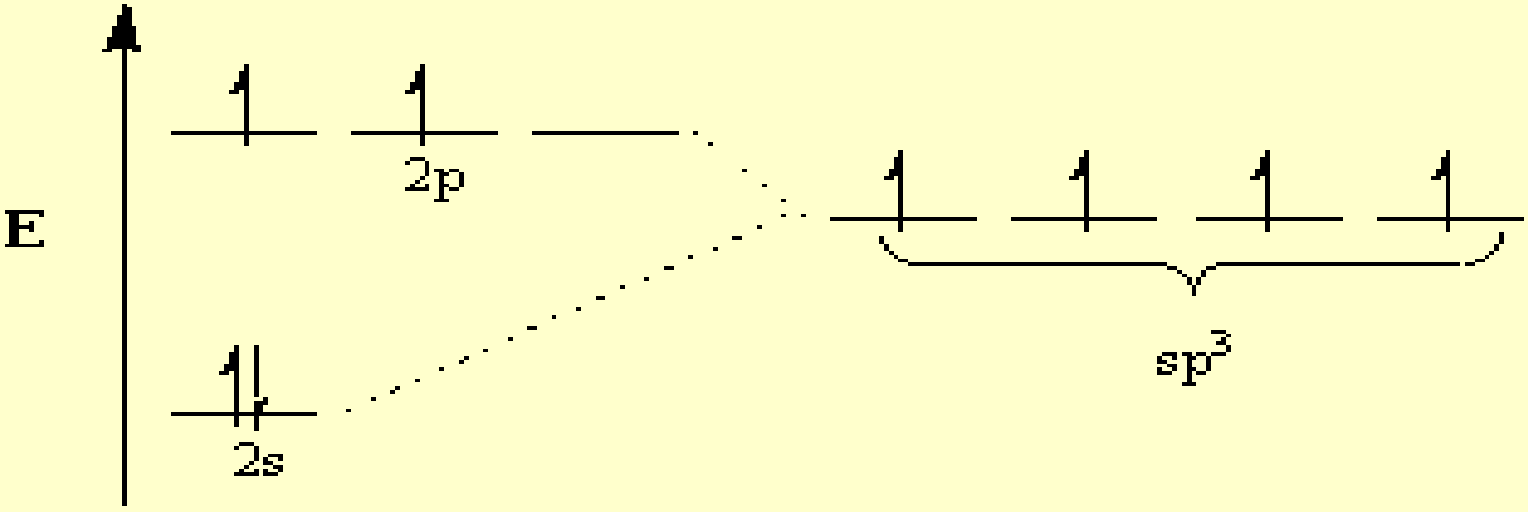
Can you draw the stable polyatomic structure for :

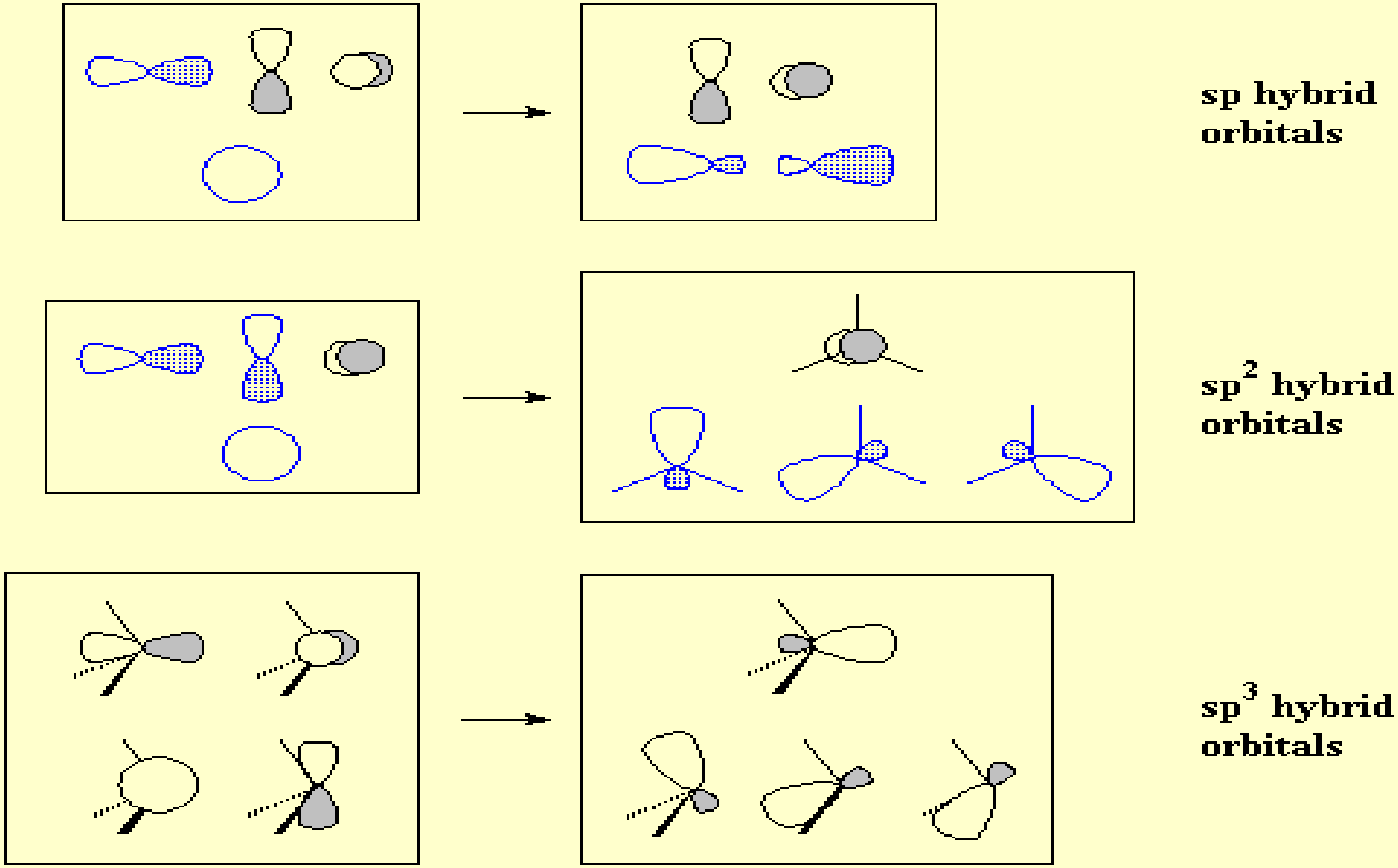
Sulfate SO_4^{-2}

Ammonia NH_4^{+}

The Hybridization of Carbon

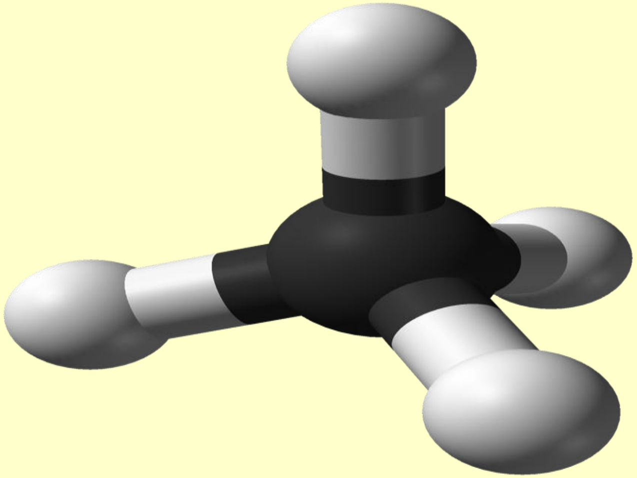
Carbon has an ability to mix the s and p orbitals and make a hybrids

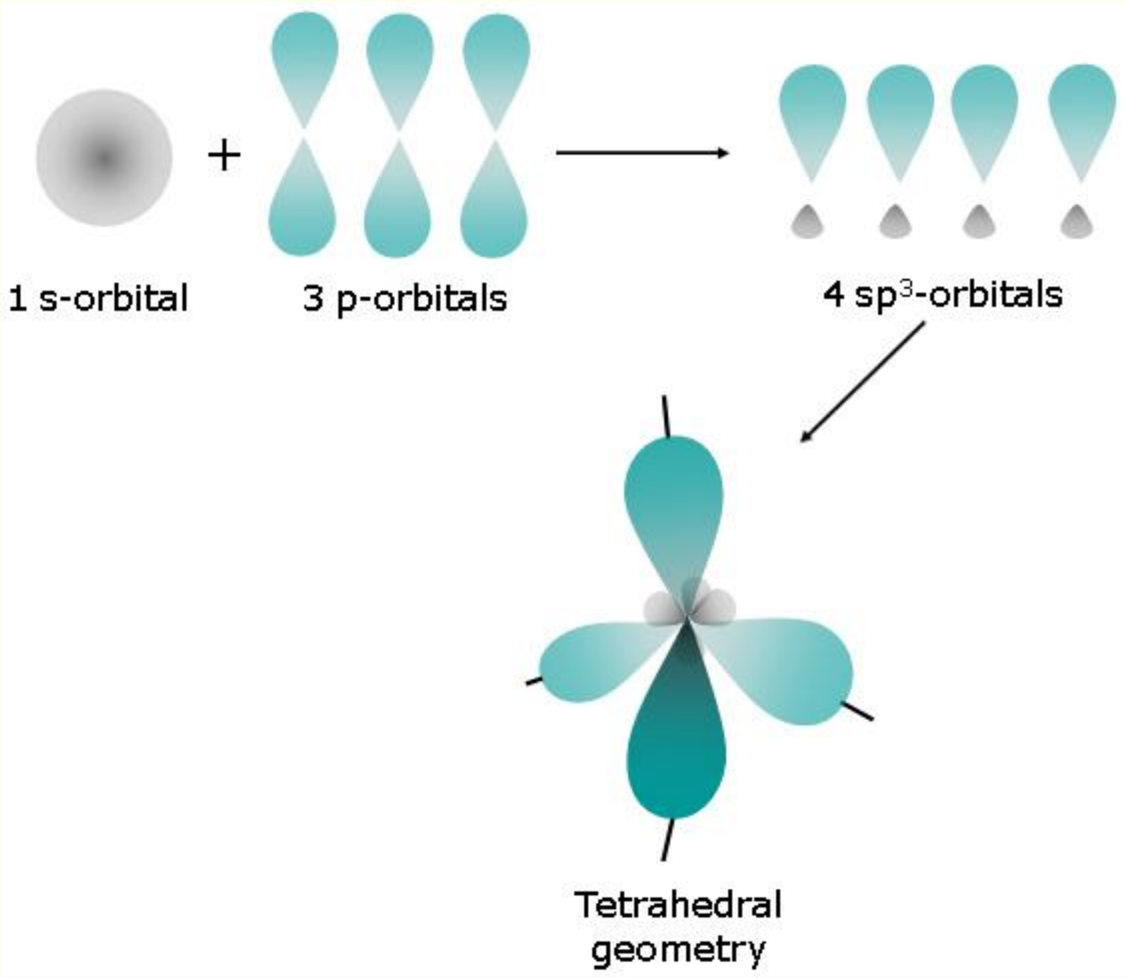




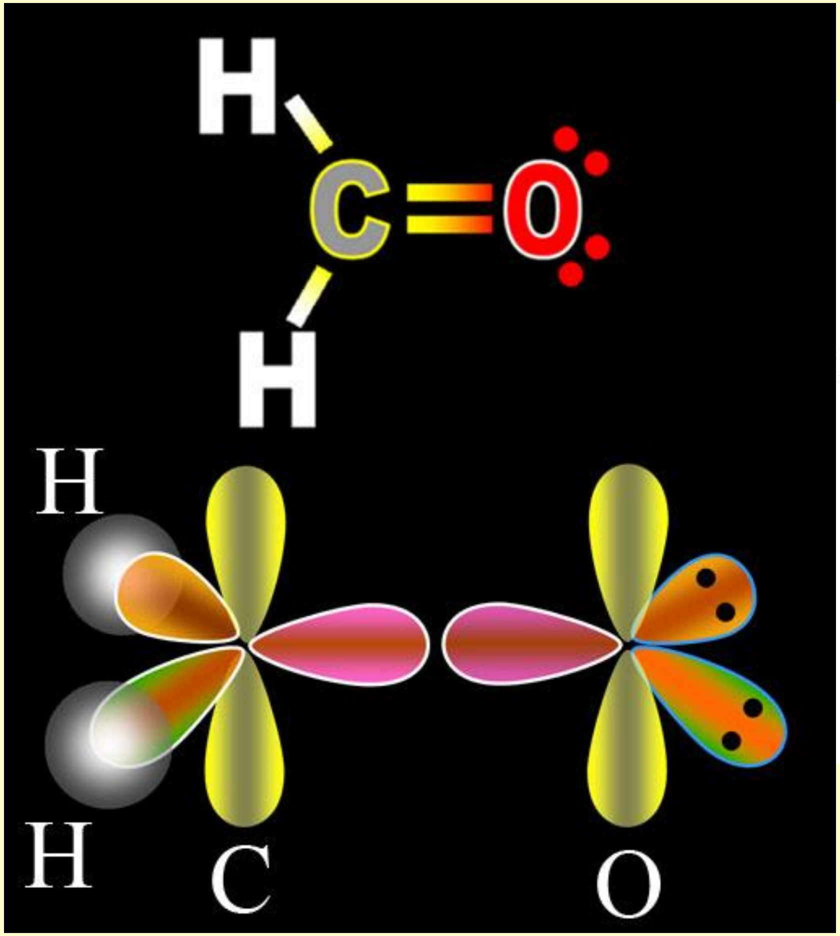
If all three are mixed 4 SP^3 orbitals are created making 4 equivalent bonding sites

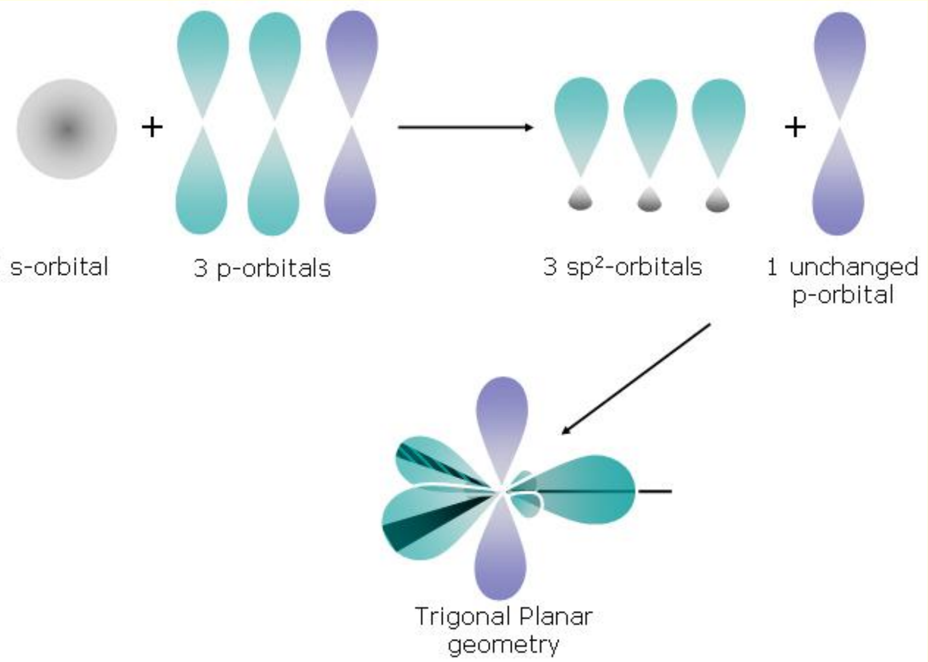
Methane – each carbon to hydrogen bond is identical



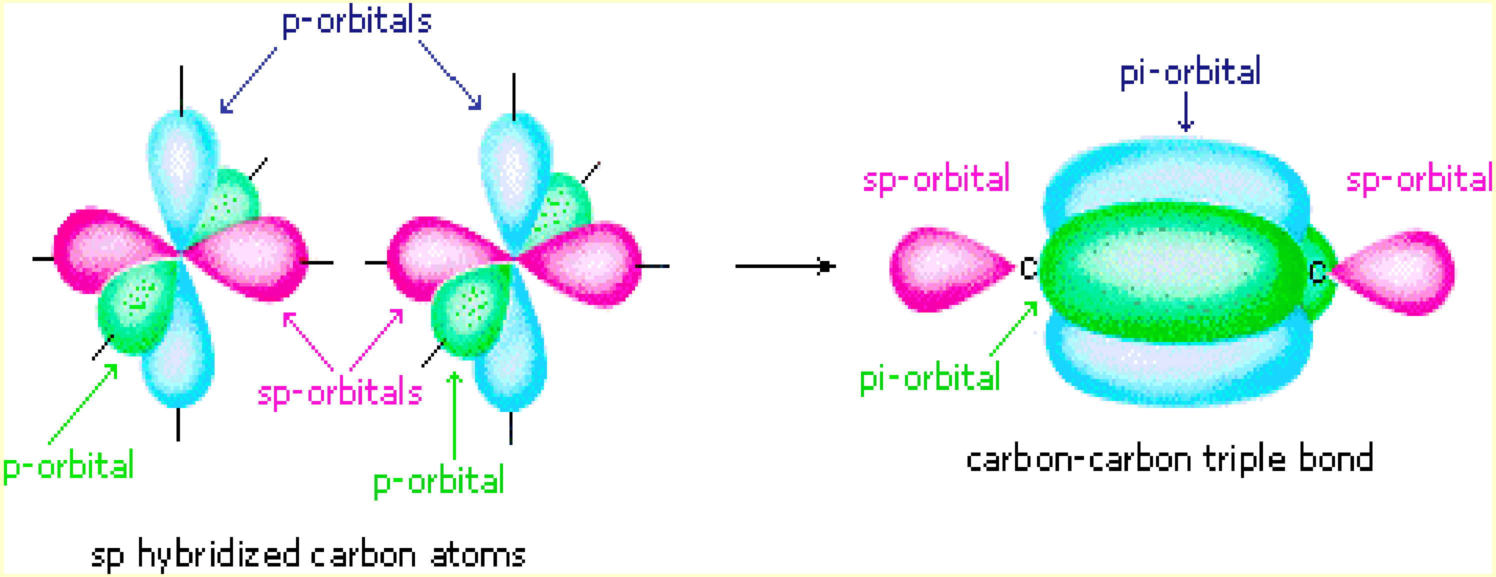


Formaldehyde CH_2O



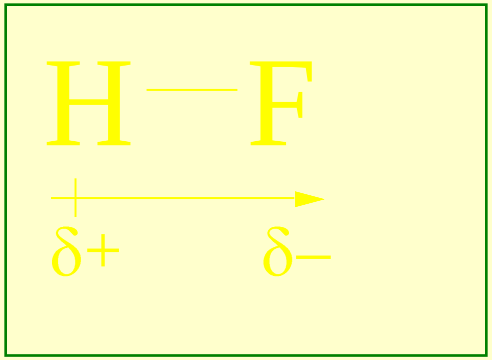


Hybridization in Ethylene C_2H_2



Polarity

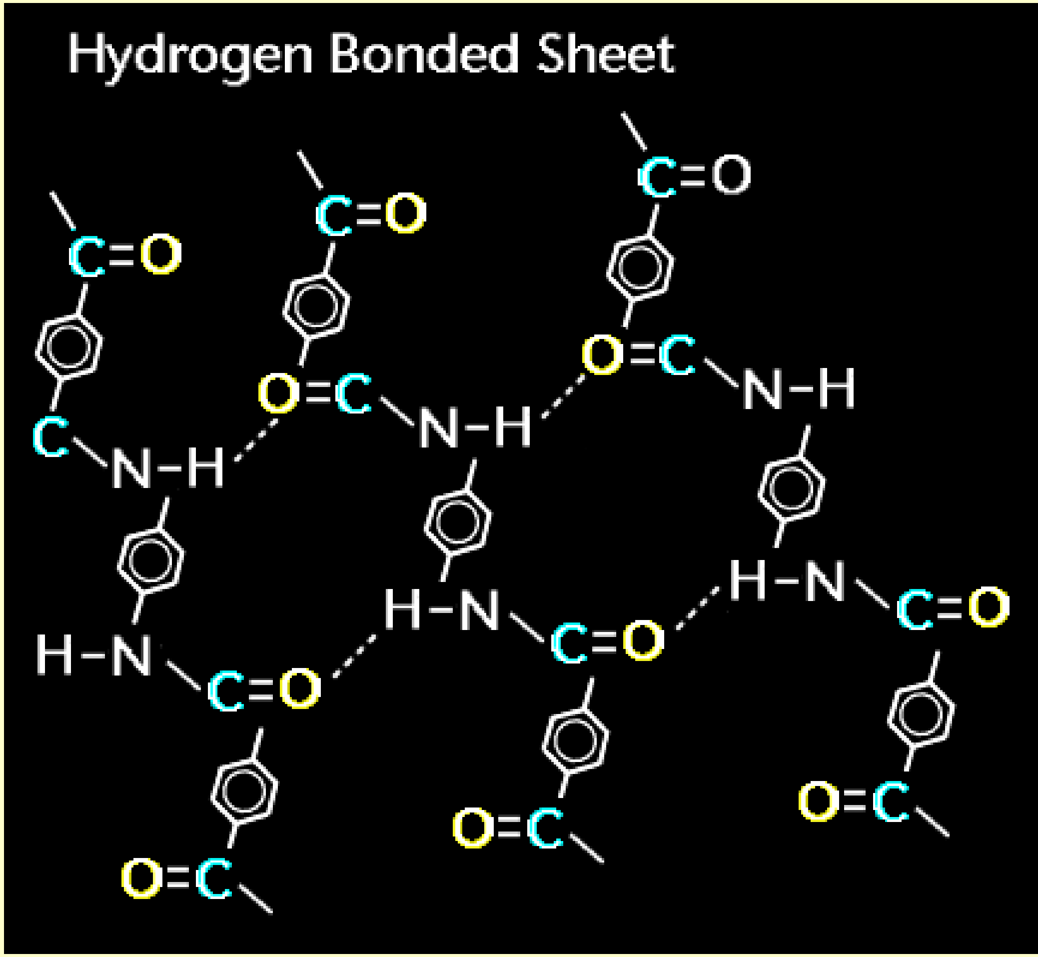
A molecule, such as HF, that has a center of positive charge and a center of negative charge is said to be polar, or to have a dipole moment.



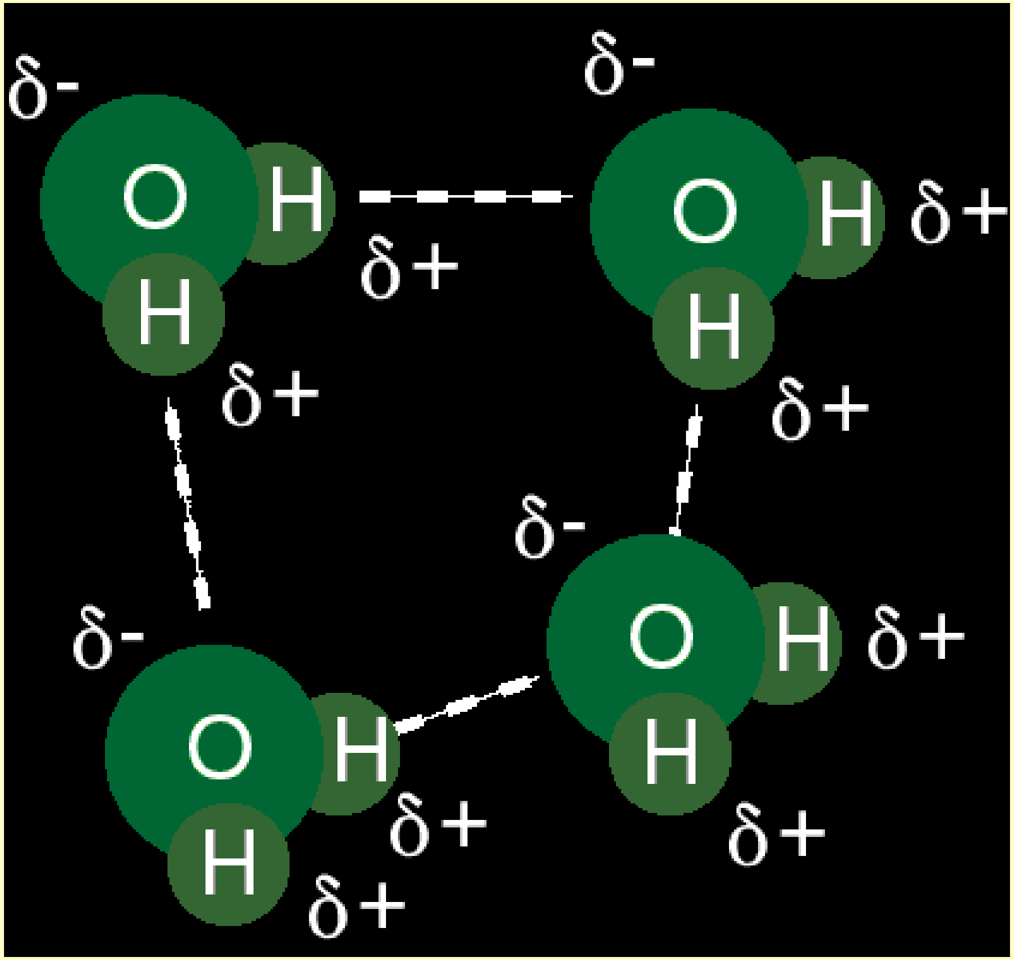
Hydrogen Bonding

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.

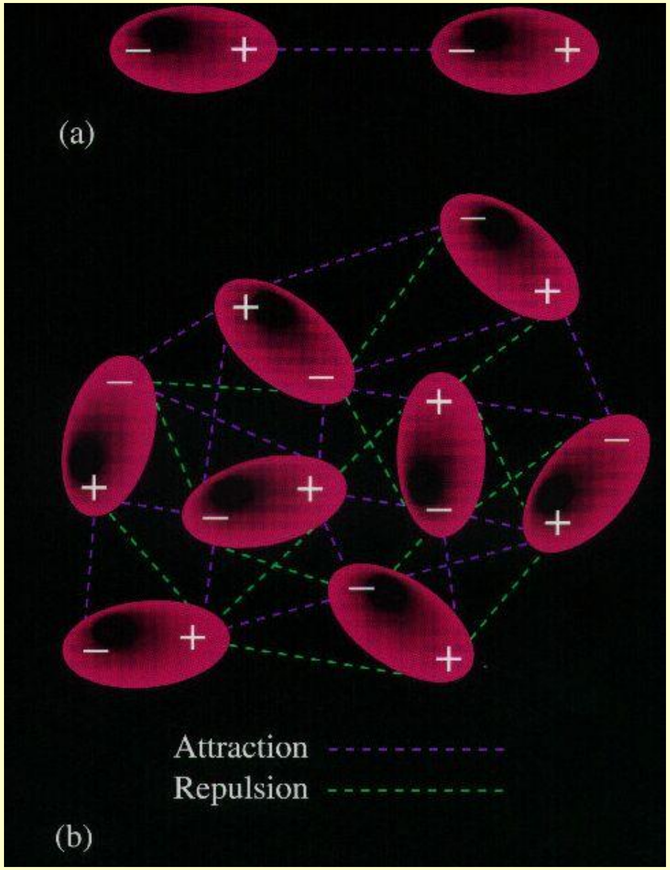


Hydrogen Bonding in Water



Dipole-Dipole Attractions

Attraction between oppositely charged regions (polar) of neighboring molecules.



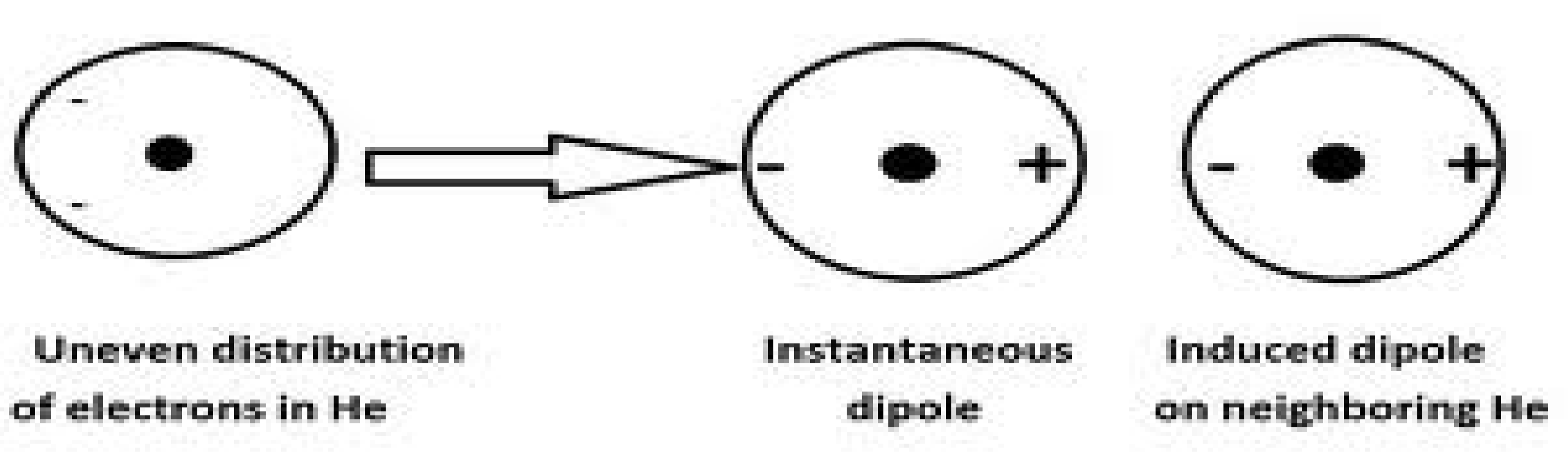
Paramagnetism

- Paramagnetism refers to a property of materials in which they are attracted to a magnetic field.

- Paramagnetism results from the presence of least one unpaired spin in the material's atoms or molecules.

London Dispersion Forces

- Weakest intermolecular force.
- a temporary attractive force that results when the electrons in two adjacent atoms/non-polar molecules occupy positions that make the atoms form temporary dipoles.
- causes nonpolar substances to condense to liquids and to freeze into solids when the temperature is lowered sufficiently.



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 Dispersion forces (less than 1 kcal)

Weakest