Ch06

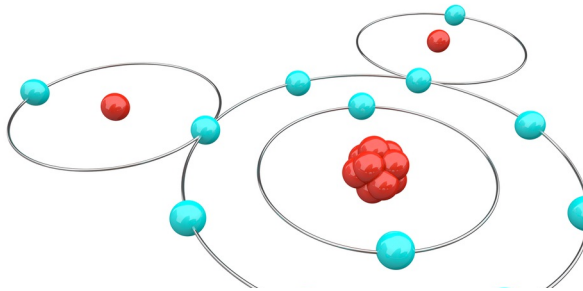
Molecules

How atoms connect to form ... everything.

"When carbon, oxygen and hydrogen atoms bond in a certain way to form sugar, the resulting compound has a sweet taste.

The sweetness resides neither in the C, nor in the O, nor in the H;
it resides in the pattern that emerges from their interaction."

— F. Capra 2002



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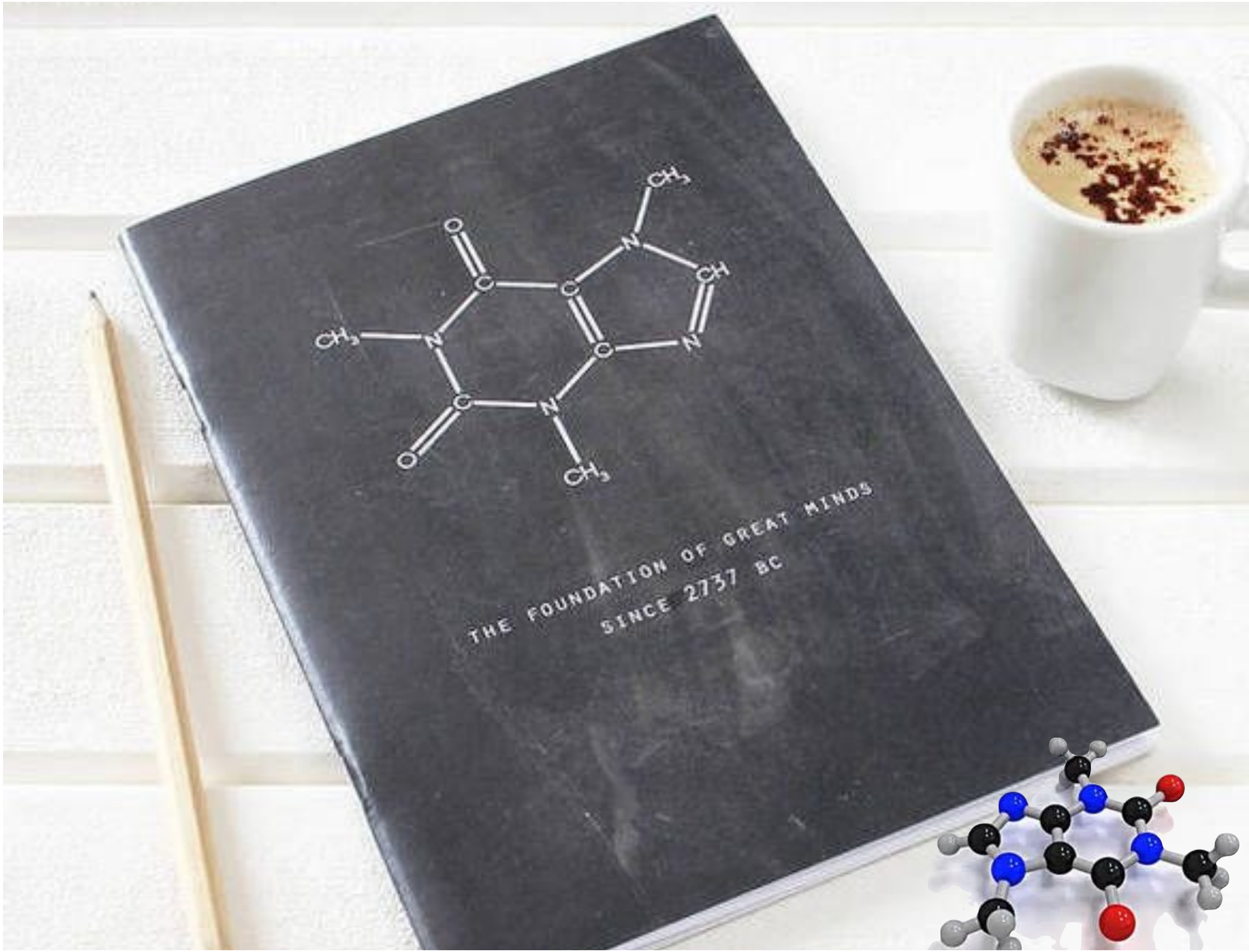
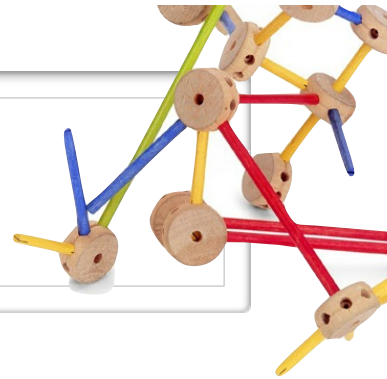

THE FOUNDATION OF GREAT MINDS
SINCE 2737 BC

Ch06

Molecules



- Understanding Molecules
  - The covalent bond.
    - Gilbert Lewis
    - Connectivity
  - Lewis Notation
    - Lewis Symbols
    - The octet rule.
    - Explaining bonding patterns.
- Electronegativity
  - Polar covalent bonds
    - Bond Dipoles
  - Pauling values
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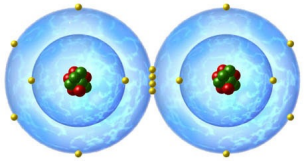
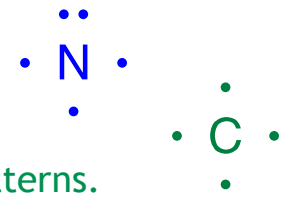
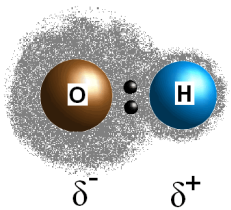
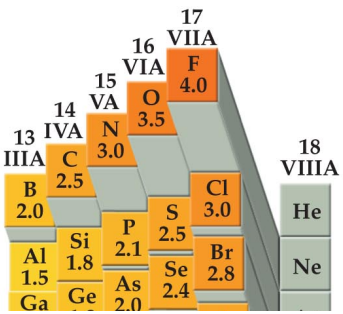
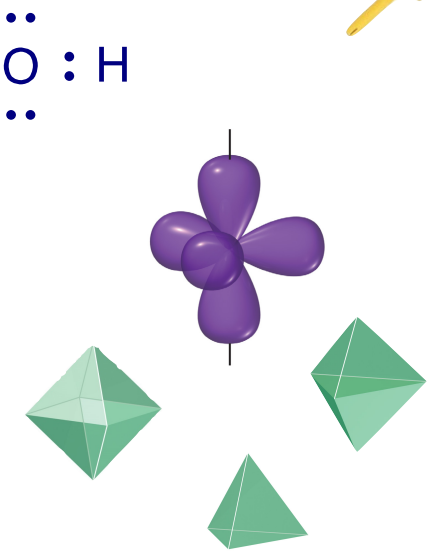


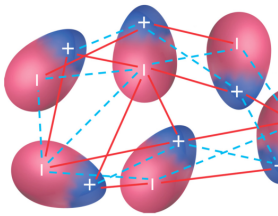


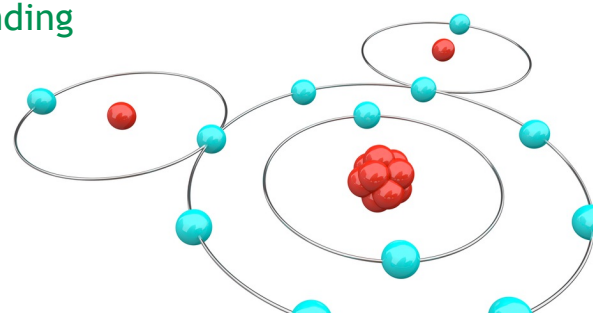




- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions
- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure
- Intermolecular Forces
  - Molecular Dipoles
  - Forces
    - Dipole-Dipole
    - London Forces
    - Hydrogen Bonding



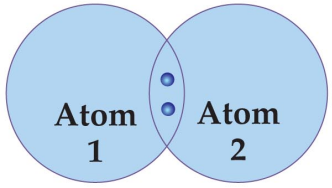




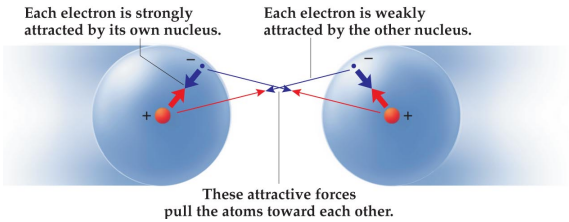
Bonding Atoms

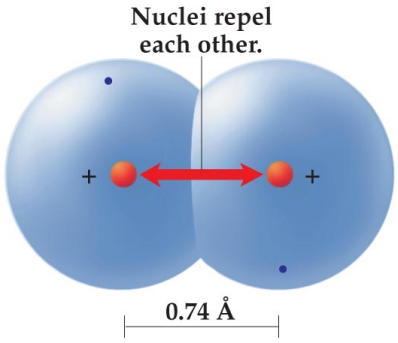
Covalent Bonding (only non-metals)

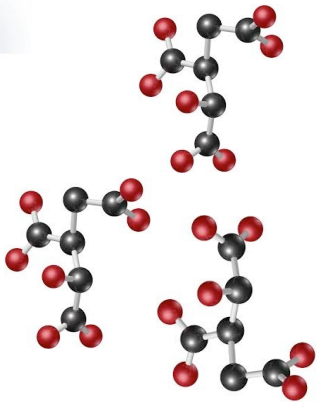
- Nonmetals pull on each others electrons.
- The shared electrons are localized between two atoms, creating a bond between just those two atoms.
- Covalent bonding produces discrete microscopic structures built of atoms.
- Particles made of covalent bonds are molecules.
- Compounds made from covalent bonds are molecular compounds.



Covalent bond:
electrons shared equally

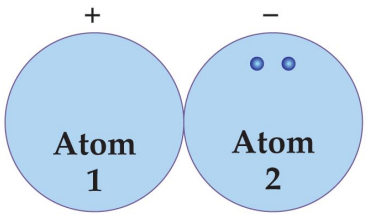




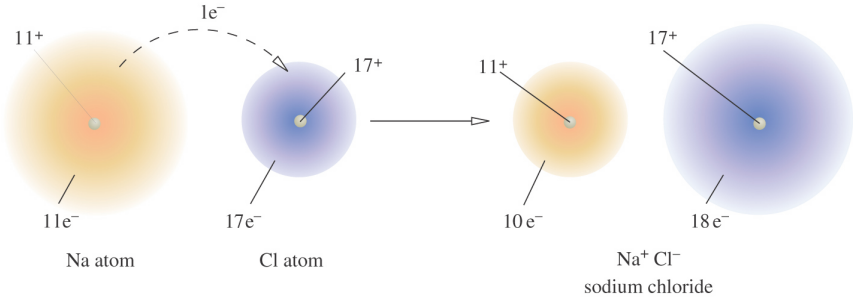


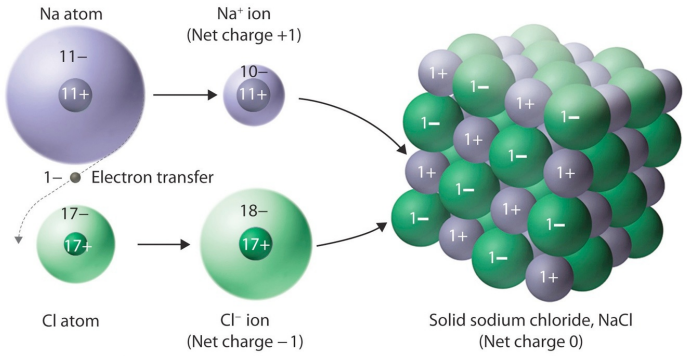
Ionic Bonding (metal with non-metal)

- Ionic bonding creates positively and negatively charged particles.
- The particles attract each other, this is an ionic bond.
- These ions clump together in simple, large complexes.
- Compounds made from ionic bonds are ionic compounds.



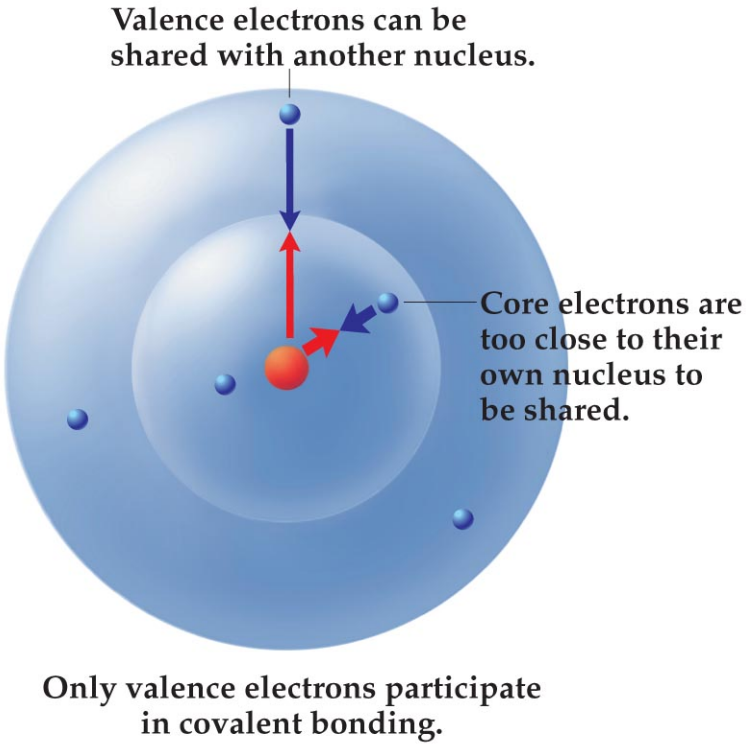
Ionic bond:
electron transferred

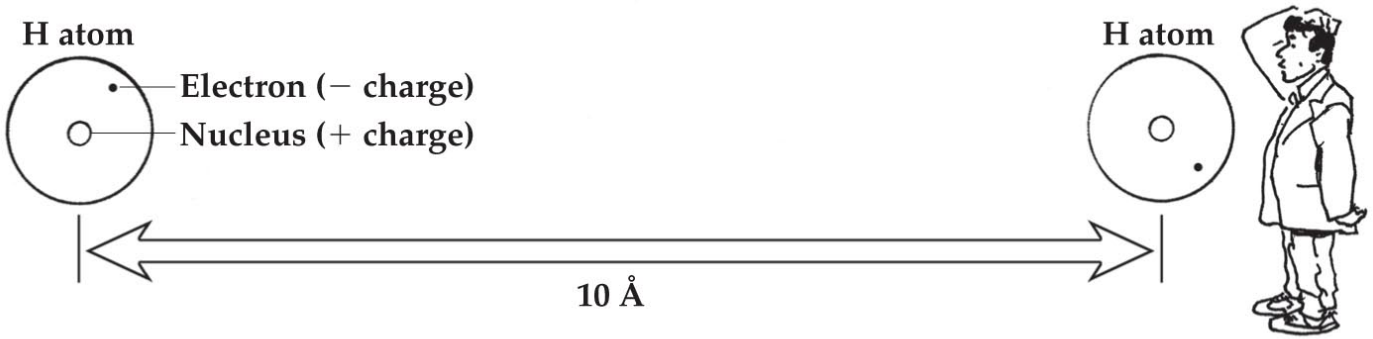




The Covalent Bond

- Thermodynamics drive bond formation.
  - Thermodynamics favors ionic bonds…
    - – when it takes less energy to rip an electron off an atom that you get back by putting it on another.
  - When that's not the case, there is still a way to satisfy atoms with strong electron affinity.
    - By sharing electrons.
- Covalent Bonding occurs between neutral atoms with strong EA.
- When these atoms get within 8 angstroms (0.8 nanometers) they begin to pull on each others valence electrons.
  - Electrons that are shielded from their own nucleus.
- Like a ball falling down hill, the atoms fall into each others e-m field.
- The atoms never meet, because as they get closer the repulsion between nucleus increases, until that energy repulsion matches the attractive energy.
- That's the bottom of the well.
- At that point the atoms lock into a fixed distance from each other, usually about an angstrom (0.1 nanometer).
- Separating those atoms, breaking that bond, requires energy.





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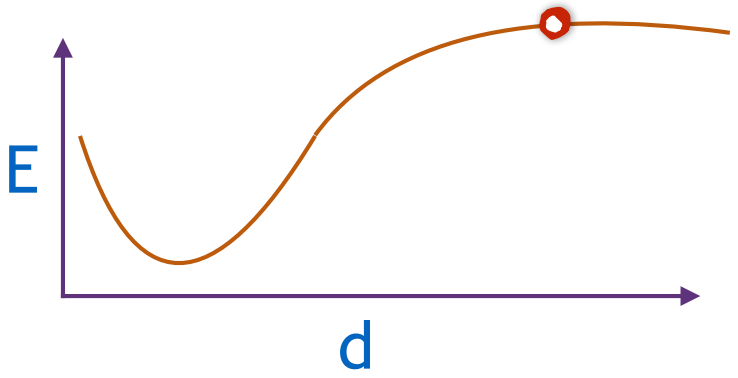

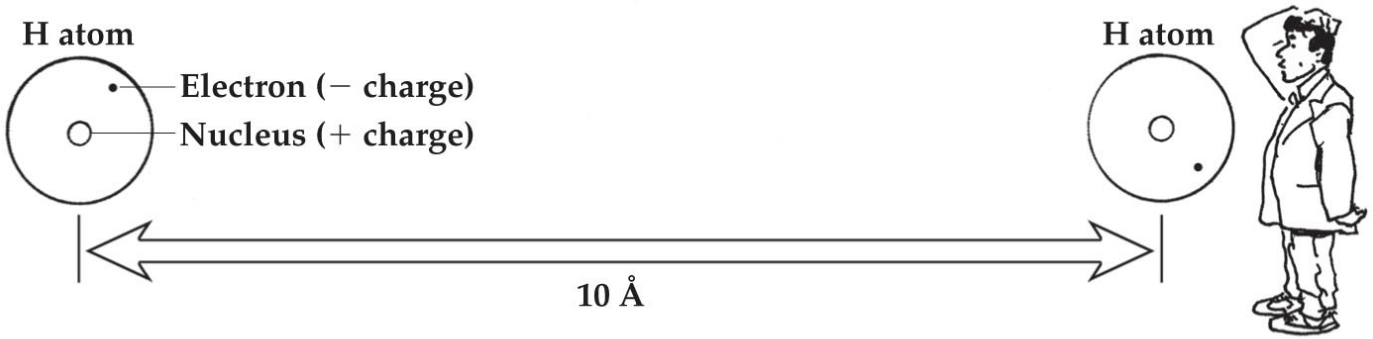

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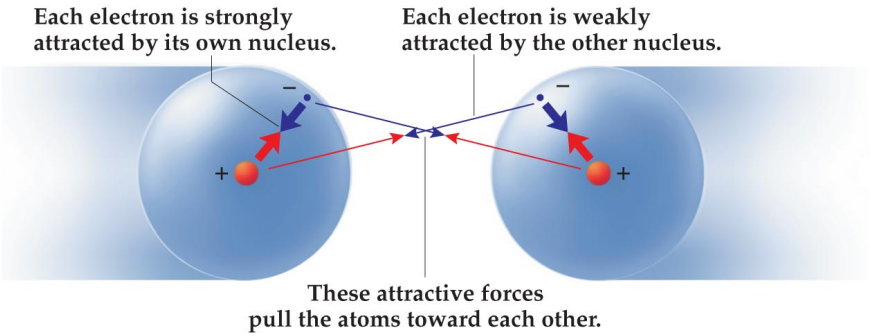

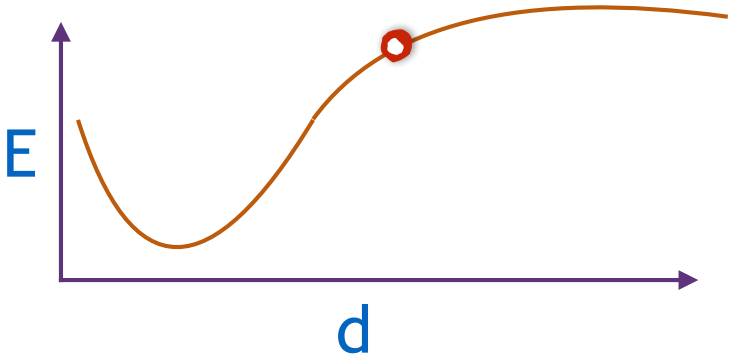

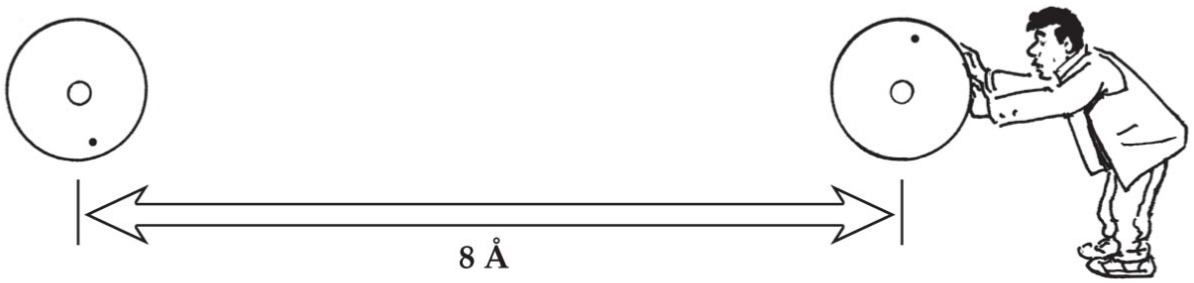

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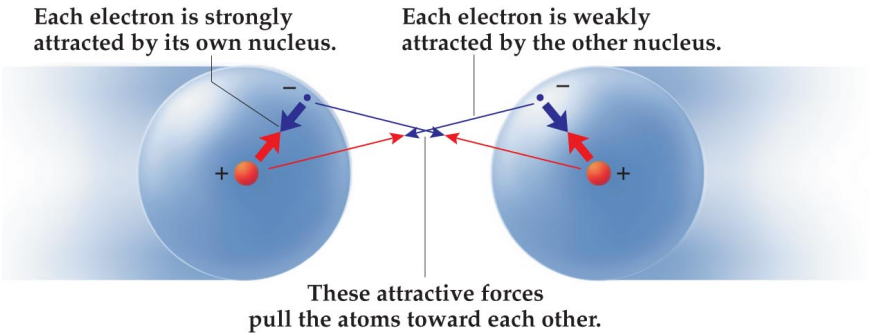

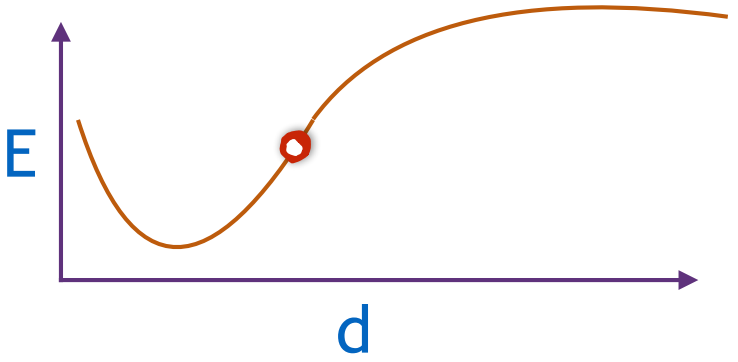

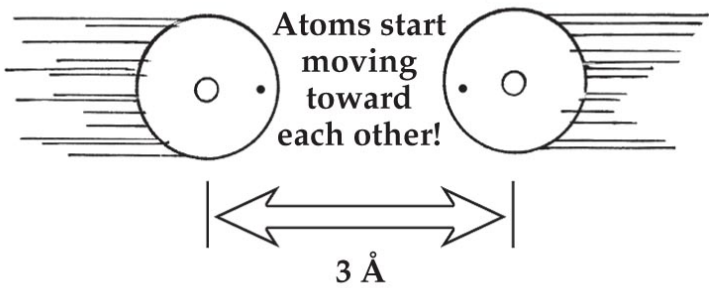

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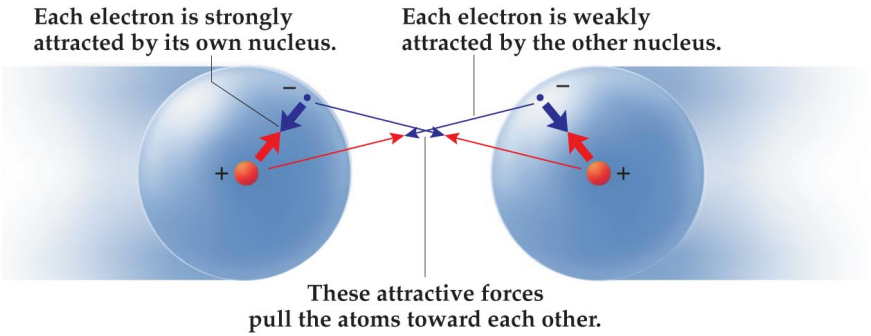

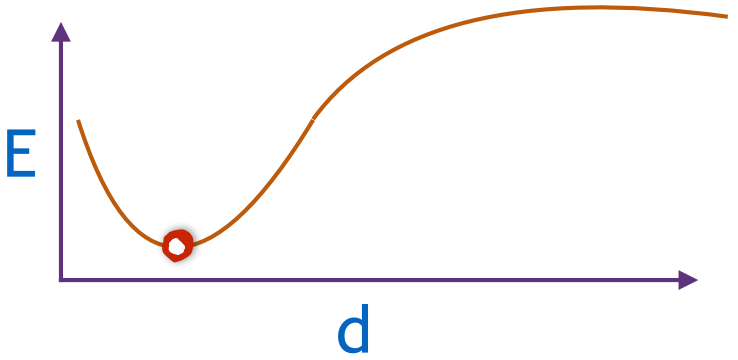

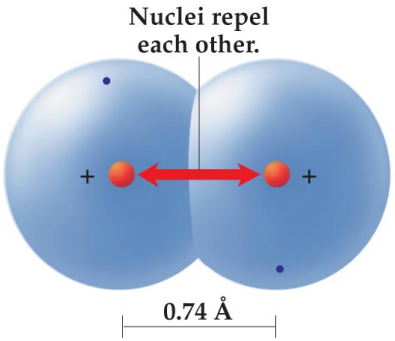

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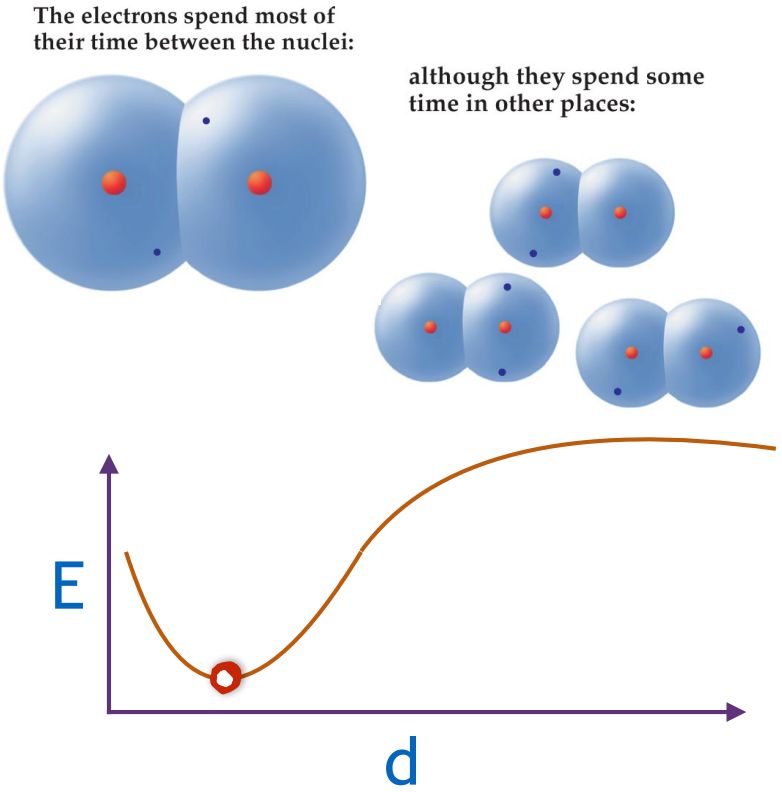
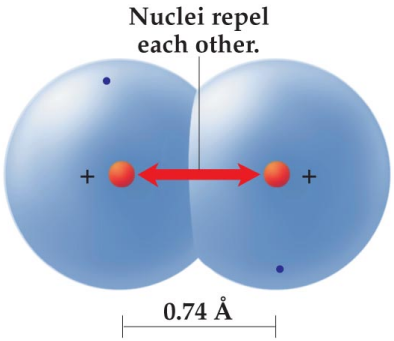
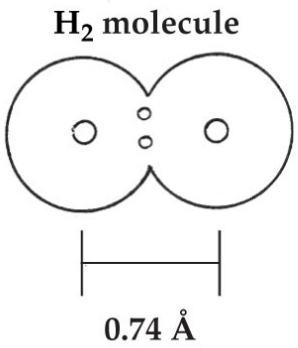
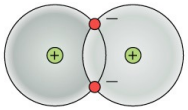






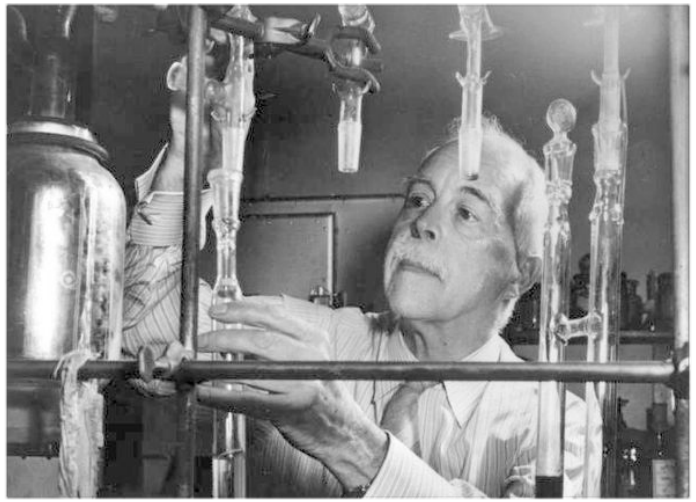
Gilbert N. Lewis

- Discovered the Covalent Bond
  - The basis for all organic chemistry.



- Coined the term Photon

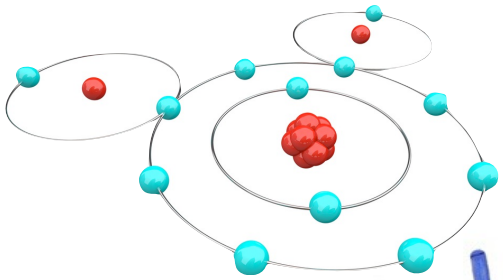
  - Although Planck and Einstein advanced the concept of quanta, Einstein did not use the word photon in his early writings and as far as my reading goes, he never did. The word "photon" originated from Gilbert N. Lewis years after Einstein's photoelectric paper and appeared in a letter to the editor of Nature magazine.
  - "I therefore take the liberty of proposing for this hypothetical new atom, which is not light but plays an essential part in every process of radiation, the name photon." -Gilbert N. Lewis, 1926
    (Nature Vol. 118, Part 2, December 18, 1926, page 874-875)

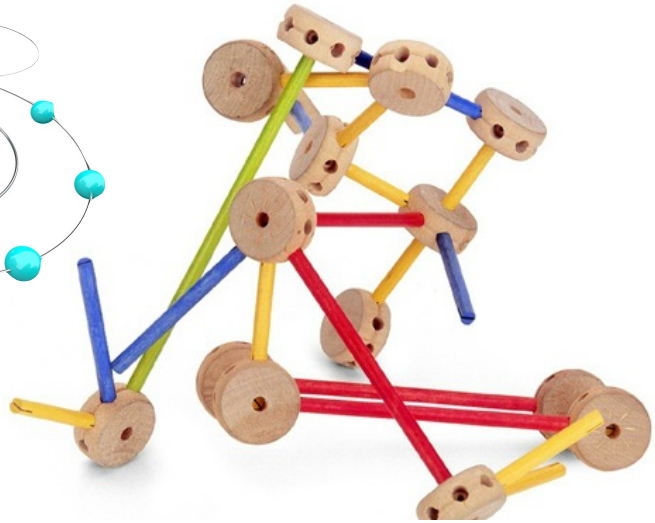


(1875-1946)

- Formalized the electron pair theory of Acids & Bases which is why we call them "Lewis Acids"
- Developed the process for purifying Heavy Water (^2H_2O)
  - Which was essential to the Manhattan project.

- Professor at UC Berkeley for 34 years
  - Lewis Hall,the Chemistry building at UC Berkeley, is named after G.N. Lewis
- Nominated for a nobel prize 35 times
  (Mahatma Gandhi was only nominated 5 times)
  - *He never received one.*
- Lewis was found dead at his lab bench at UC Berkeley in 1946, his death may have been due to poisoning from chemicals in his experiment. The coroner listed it as a heart attack.
- Developed Valence Shell Notation
  - more commonly known as Lewis Dot Structures





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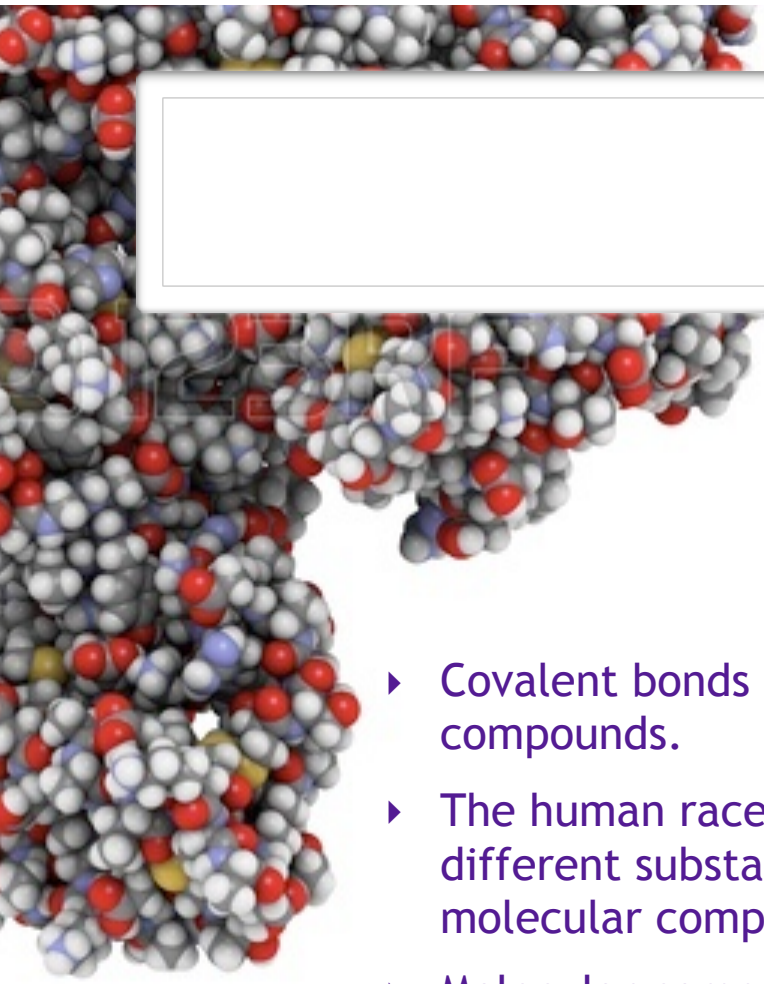
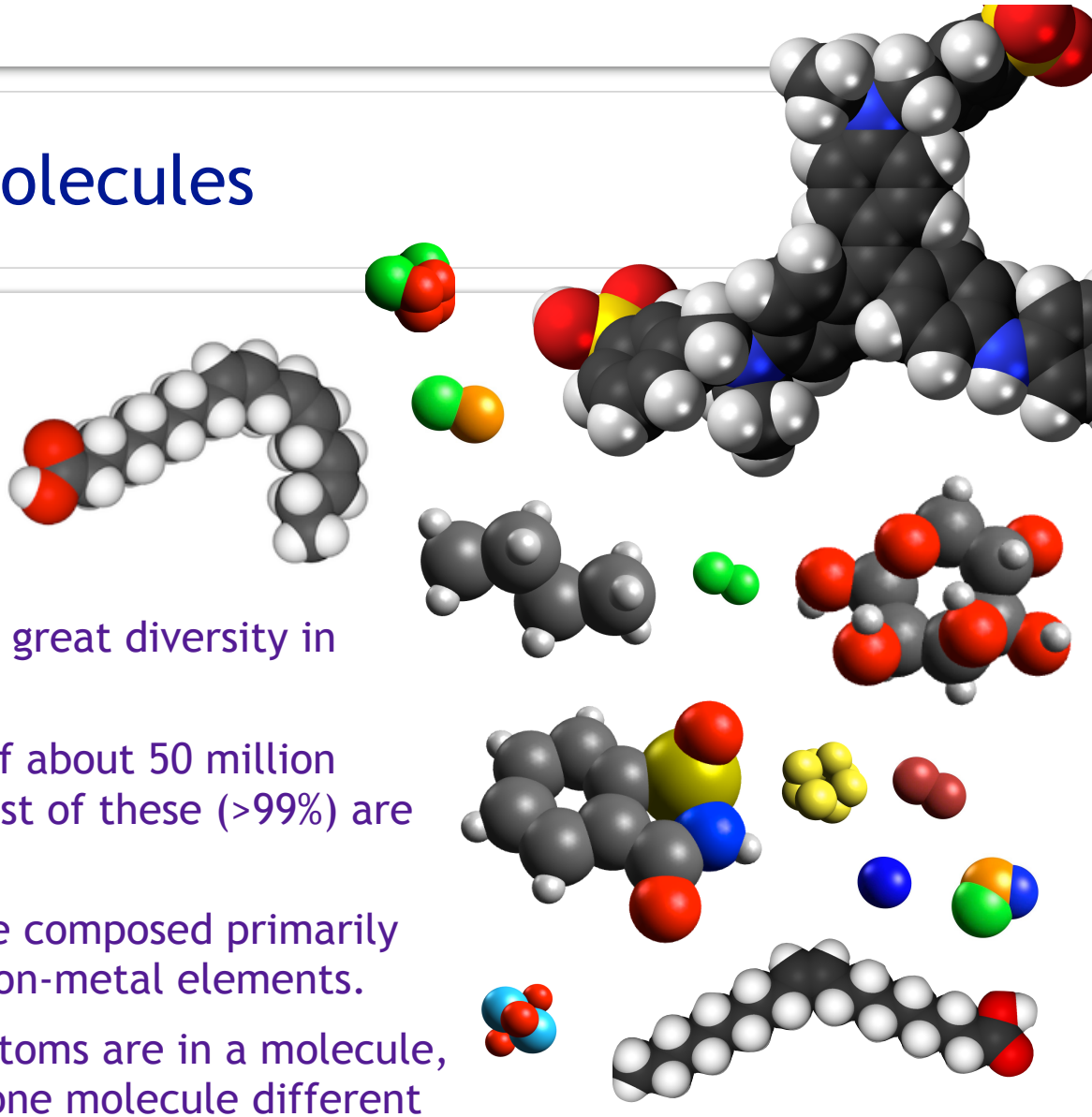
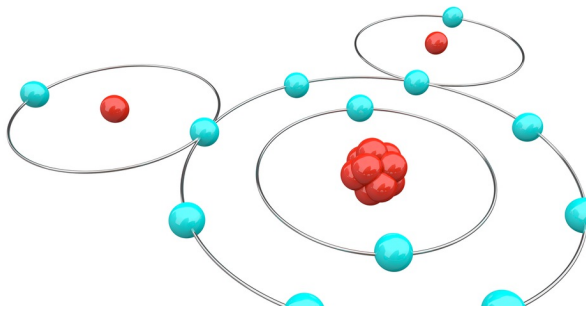




- Covalent bonds allow for great diversity in compounds.
- The human race knows of about 50 million different substances, most of these (>99%) are molecular compounds.
- Molecular compounds are composed primarily (almost exclusively) of non-metal elements.
- The composition, what atoms are in a molecule, are part of what makes one molecule different than another.
- The connectivity, which of those atoms are connected to which, are another way one molecule can be different from another.
- Covalent bonds let us make these connections.



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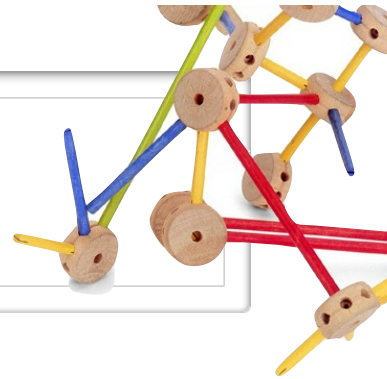

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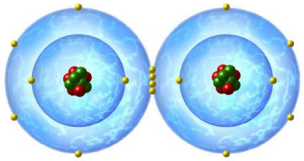
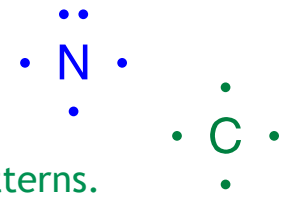
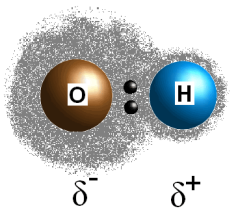
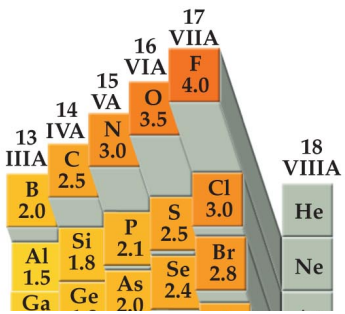
      - ionic, ΔEN = 2.0+



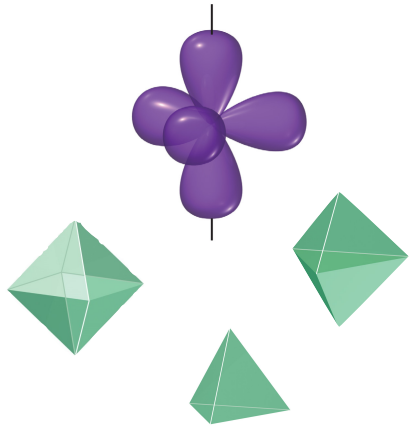






- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure



- Intermolecular Forces
  - Molecular Dipoles
  - Forces
    - Dipole-Dipole
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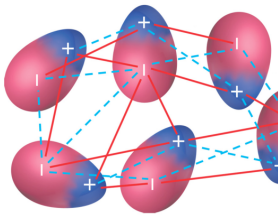
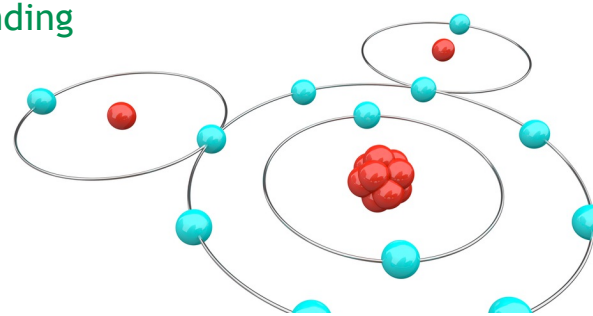




A model for understanding connectivity.

Composition

(What's in it.)

CCl_4

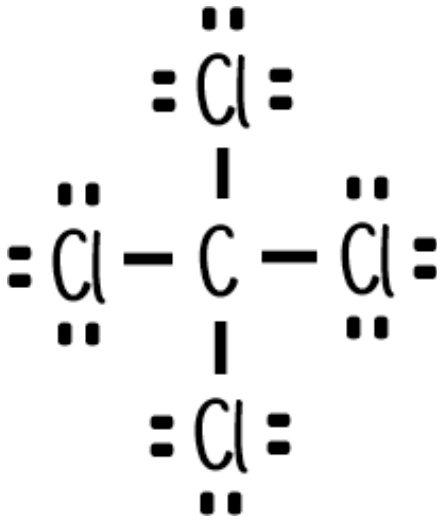
1 Carbon
4 Chlorine

Chemical Symbols

Molecular Formula

Connectivity

(What's connected to what.)



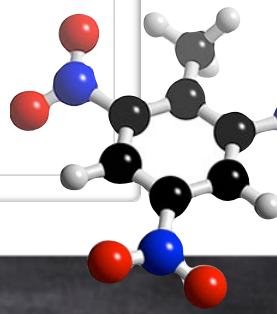
Lewis Dot Structure

Shape

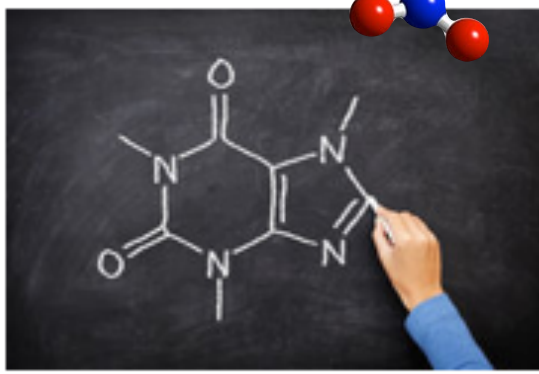
(Bond Angles & Distances)

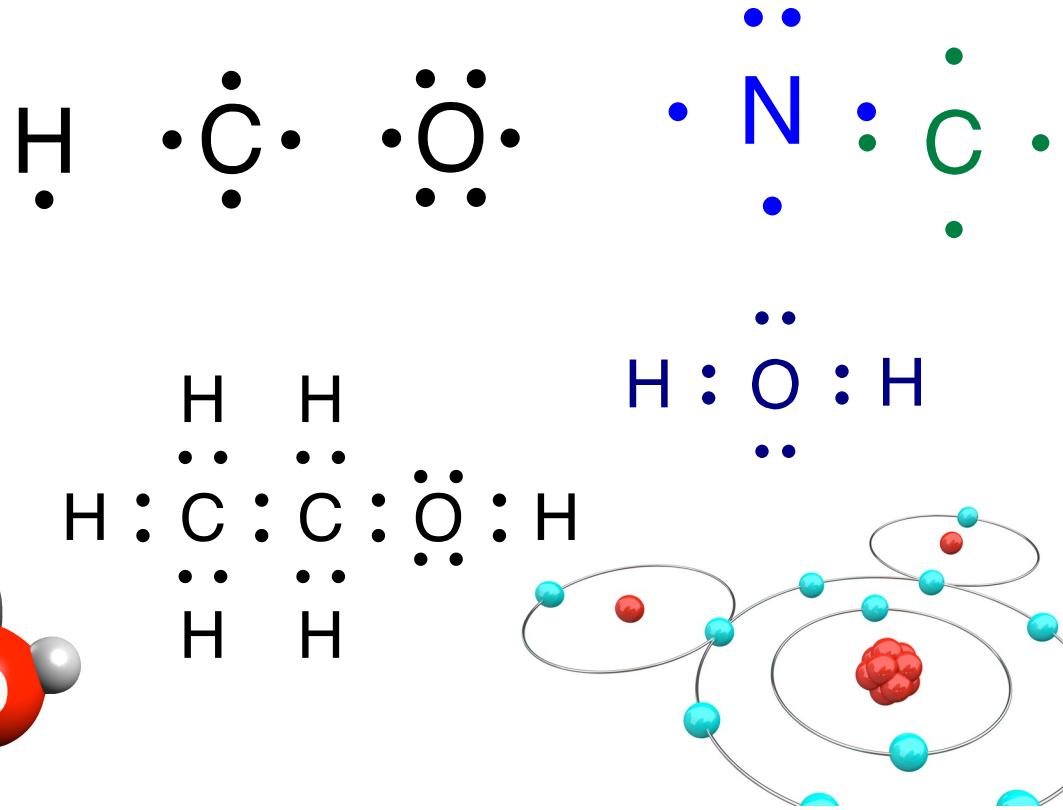
(coming up)

It starts with Lewis Symbols



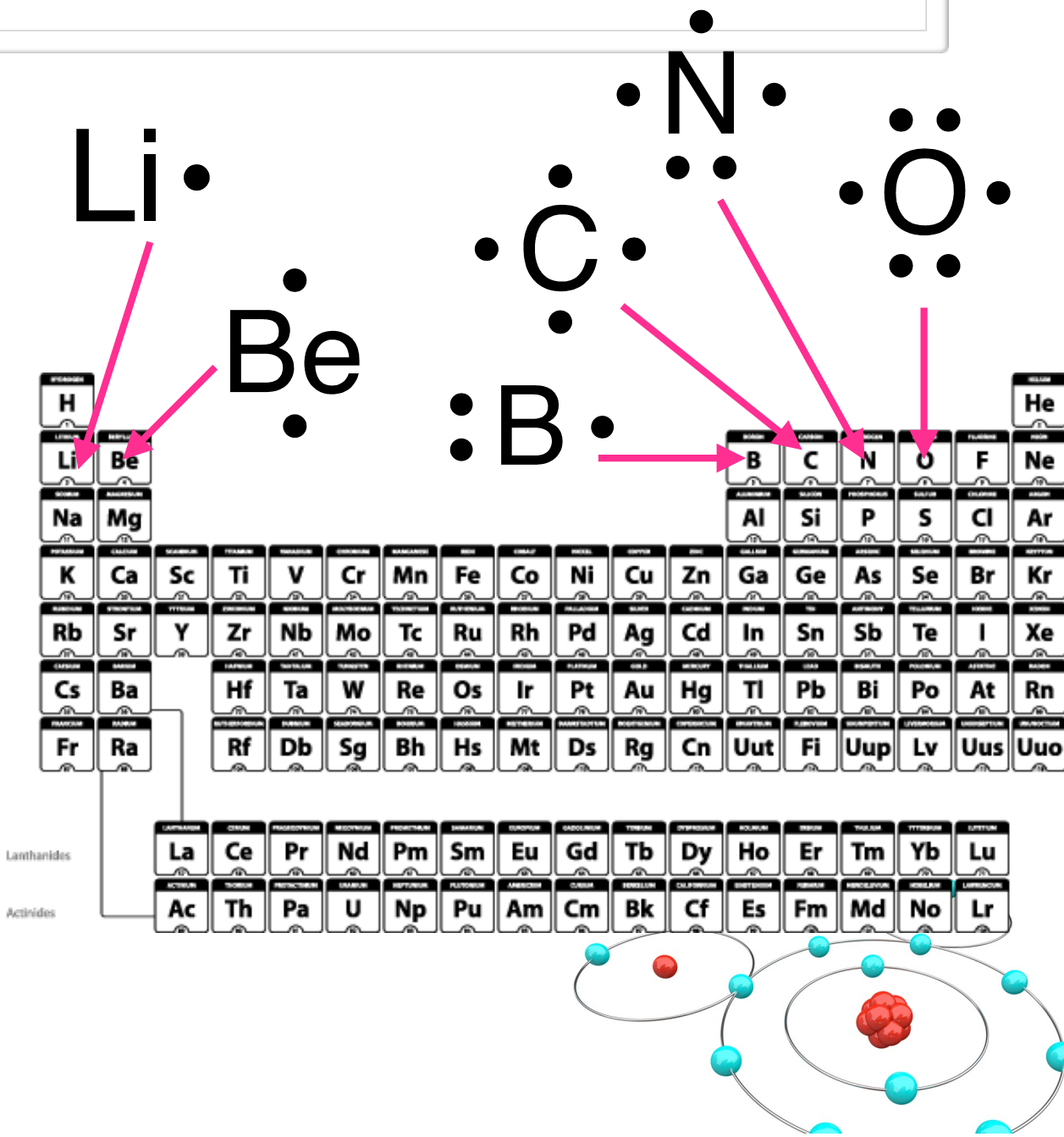
- Lewis notation is how we described the connectivity of all covalent compounds (molecules).
- It's how we understand differences between compounds even when they have the same composition (molecular formula).
- Lewis notation starts with understanding the Lewis symbols for each atom or ion.



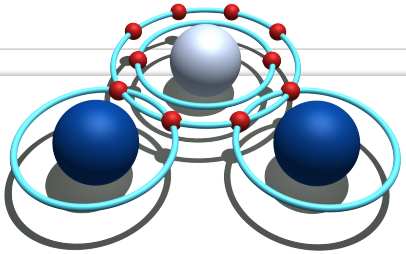


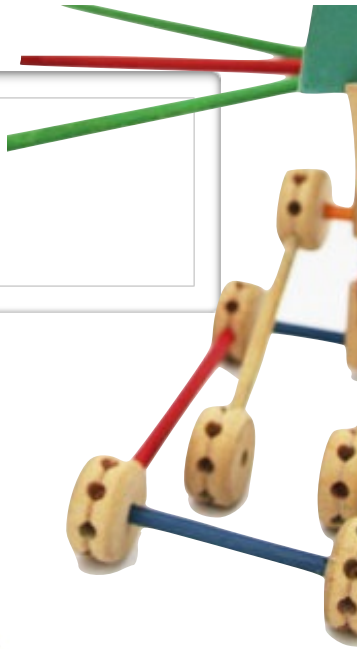
Lewis Dot Symbols

- Lewis dot symbols show only the valence electrons (electrons in the outermost shell).
- These 1-8 electrons are shown as dots or pairs of dots on four sides of the symbol.
- The order doesn't matter, as long as you put no more than two dots on a side any arrangement of dots is the same symbol.
- You know the number of valence electrons for any neutral atom, by it's location in the periodic table.
  - Group 1 elements (Li, Na, K…) have one valence electron.
  - Group 2 elements (Be, Mg, Ca…) have two valence electrons.
  - B, Al, Ga… have three.
  - C, Si, Ge… have four.
  - N, P, As… have five.
  - O, S, Se… have six.
  - F, Cl, Br… have seven.
  - Ne, Ar, Kr… have eight.

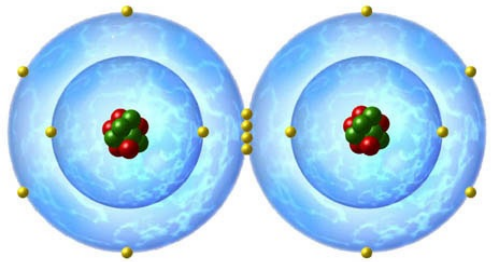


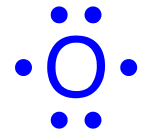
The Octet Rule

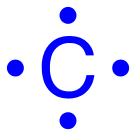


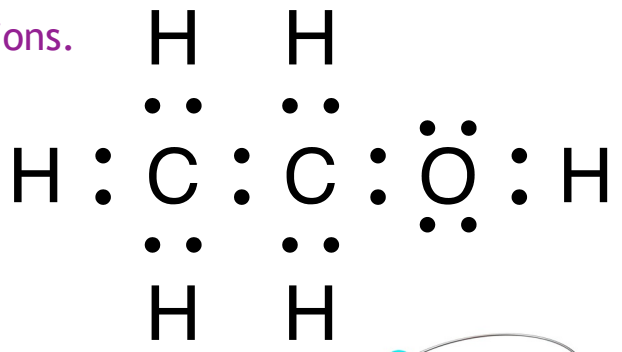


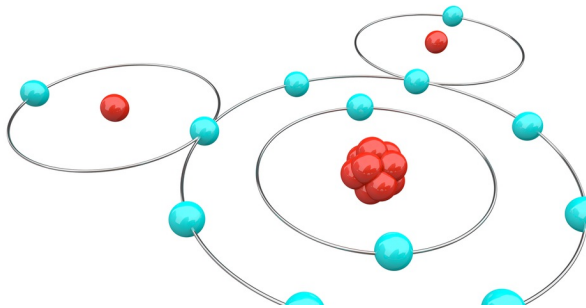
- A full valence shell is a plateau in energy.
  - There's a considerable gain in energy by reaching a full shell.
  - There's little gain in trying to add more electrons.
- The valence shell for all main group atoms (for this class we will say all atoms) have between 1-8 electrons
- The octet rule:
  - Most elements want 8 electrons in their valence shell.
- Lewis structures accurately predict chemical bonding by simply trying to fill the octet of each element by sharing or transferring electrons.
  - It's a very simple model that gives very good predictions.
  - There are exceptions to the octet rule:
    - Some elements prefer less than a full octet.
      - H, He, Al, and B are the most common.
    - A few elements have an expanded octet.
      - This can only happen in the 3rd period and below.
    - If a molecule has an odd number of electrons, someone ends up with 7.
      - 7 is the "second best" to 8, never 5 or 1 or 9 or anything else





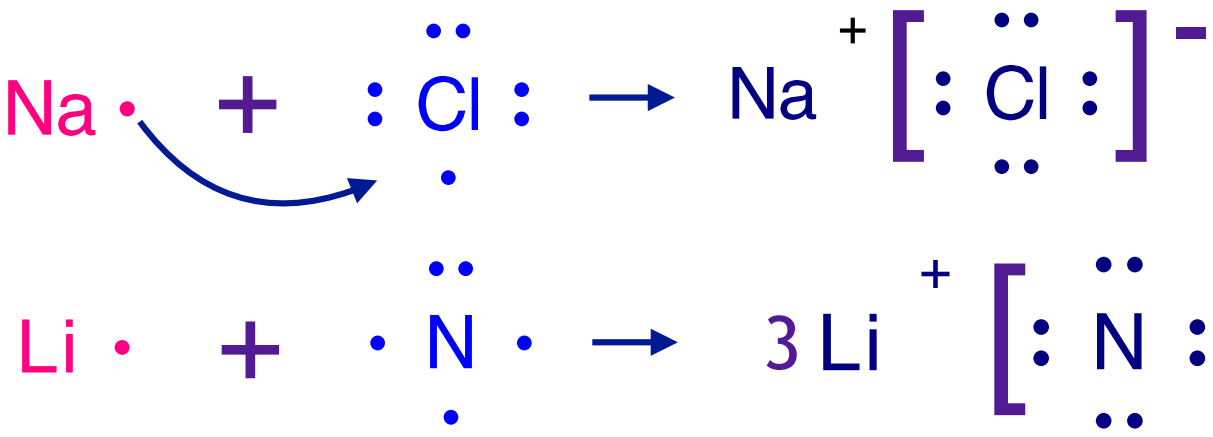






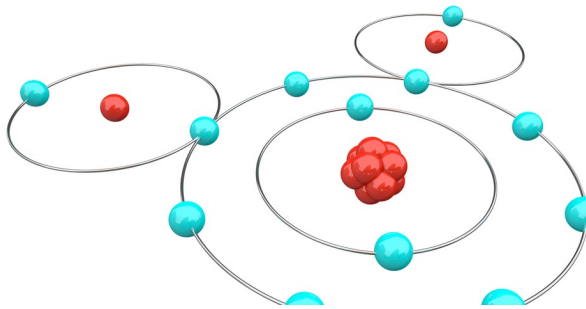
Ionic Bonding

- Lewis symbols can be used to show the structure of ions and ionic compounds.
- Ions & ionic compounds can be predicted by the octet rule.
- Elements with low ionization energy become cations.
- Elements with high electron affinity become anions.
  - Use square brackets when showing the charge of any atom or molecule that has extra electrons.
- Lewis symbols identify the chemical formula of ionic compounds.



NaCl

Li_3N



Lewis Molecular Structures

- Lewis symbols provide a simple way of visualizing and predicting covalent bonds.
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  - Shared electrons are held by both nuclei.
  - Sharing electrons allows each atom to fill it's valence.
  - The Lewis symbols allow you to predict how many electrons each atom needs and can offer.
  - The octet rule let's you know when each atom has realized a stable shared configuration.
- Electron pairs not involved in bonding are called lone pairs.
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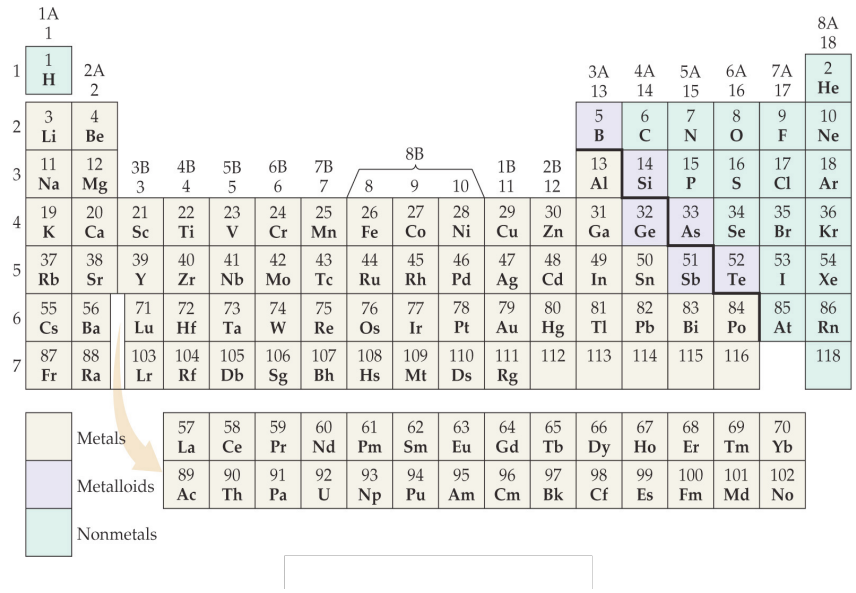
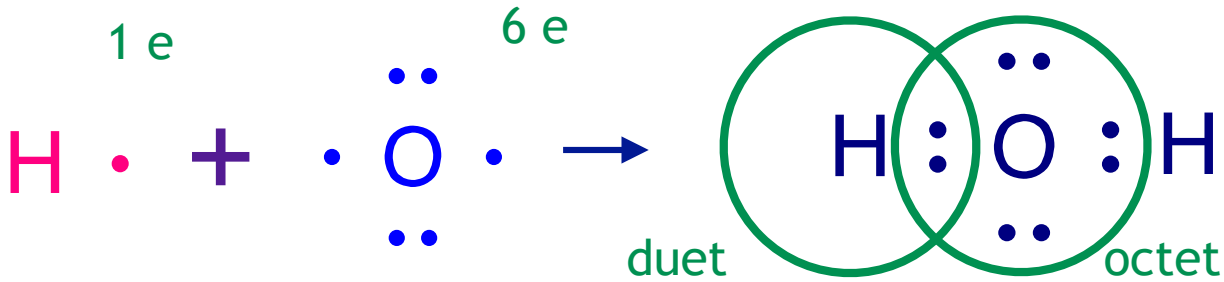
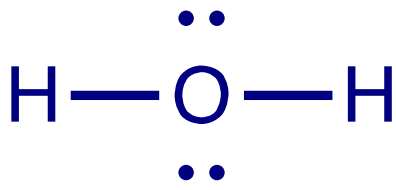
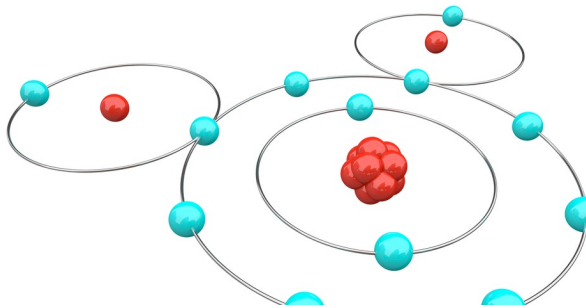
  - Bonding pairs may be replaced with a single line.
- Main group elements can form one, two, or three covalent bonds.









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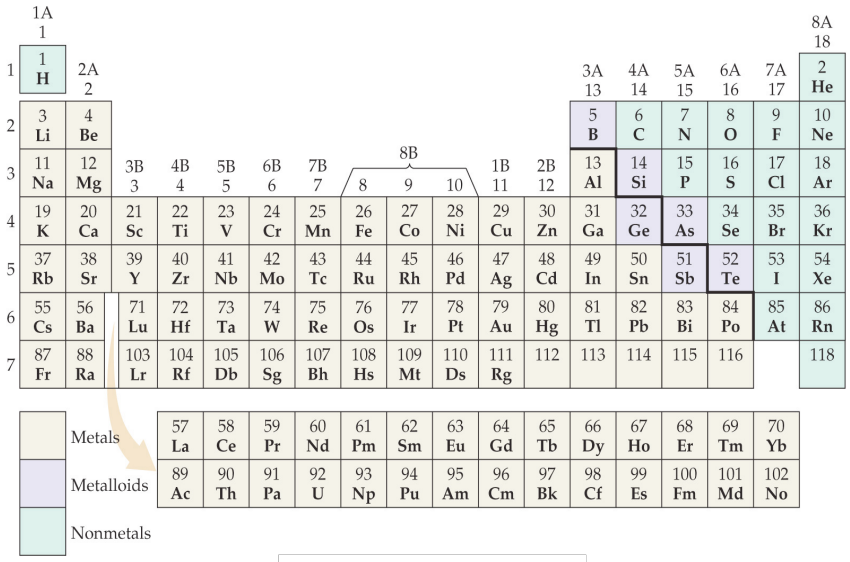

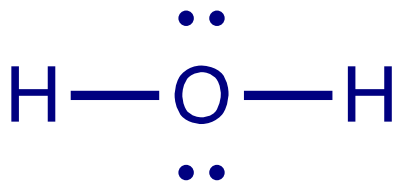

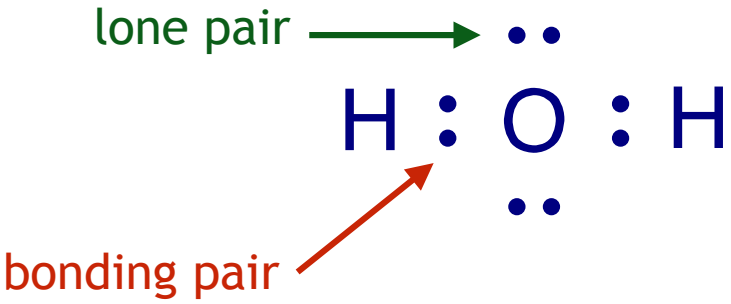

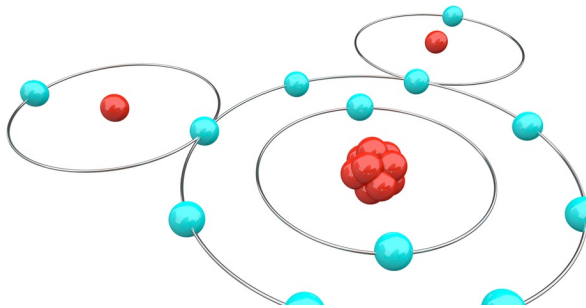

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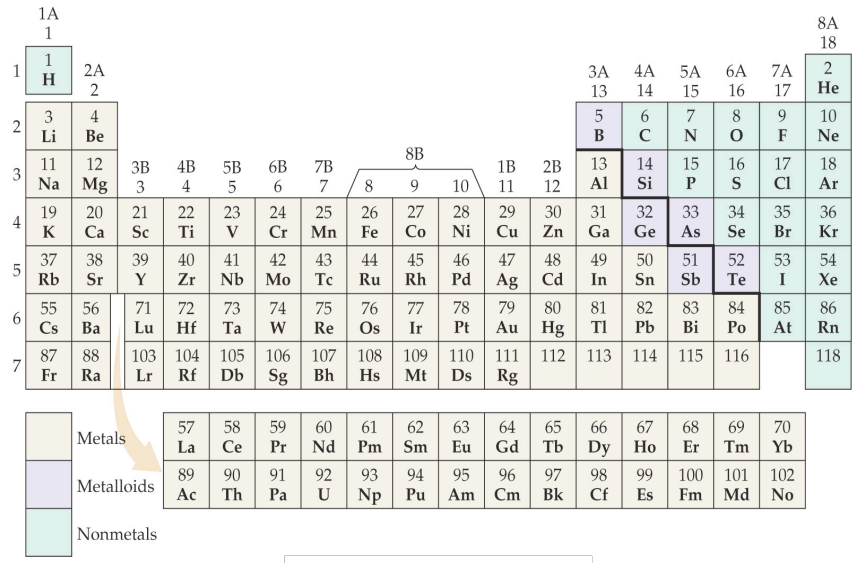

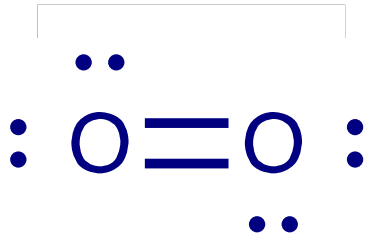

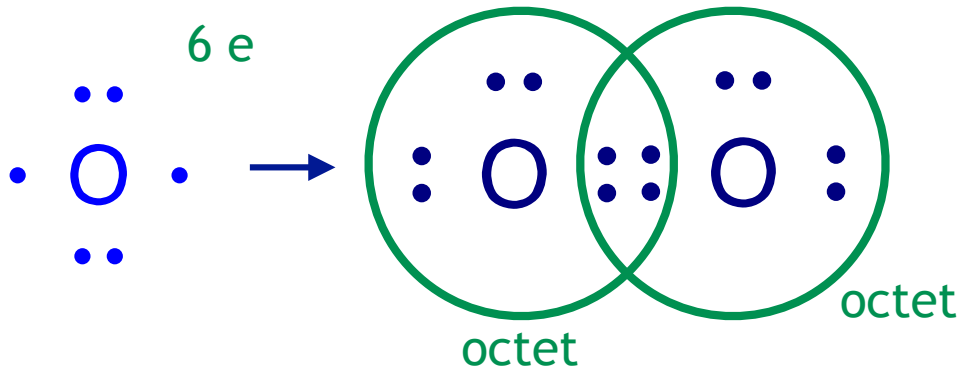

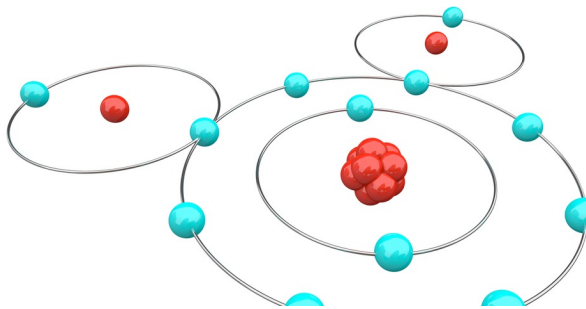

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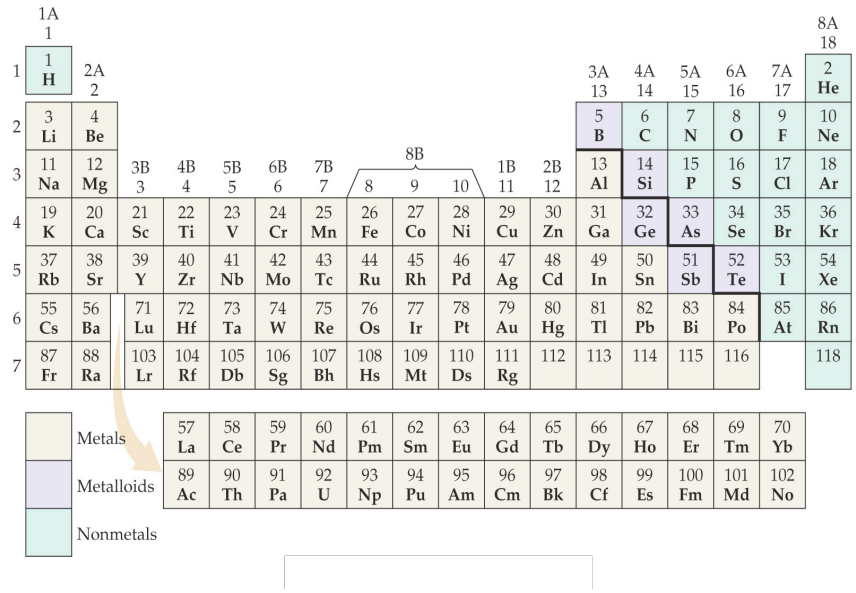
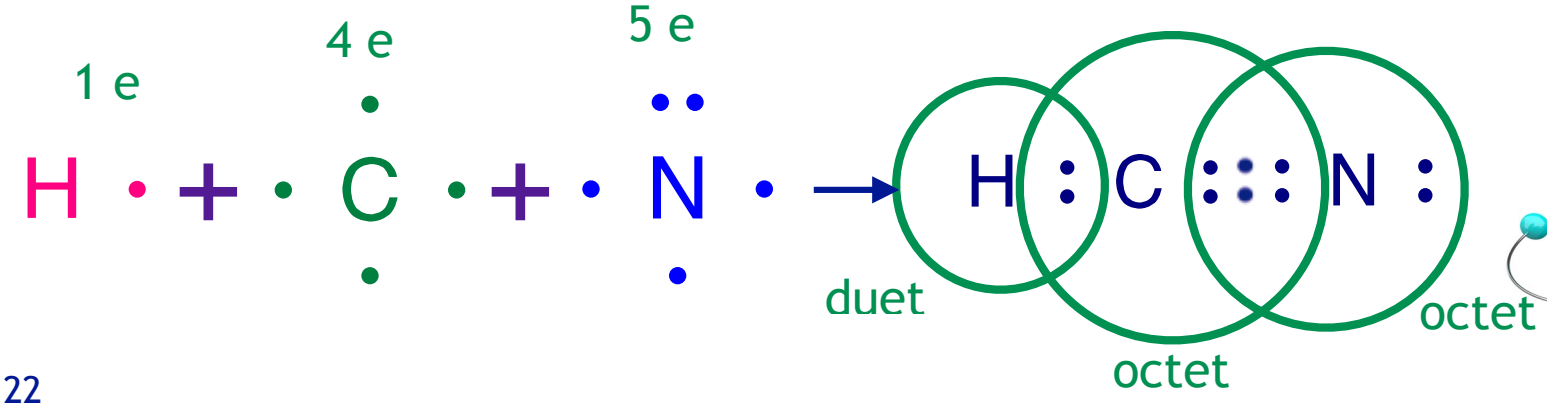
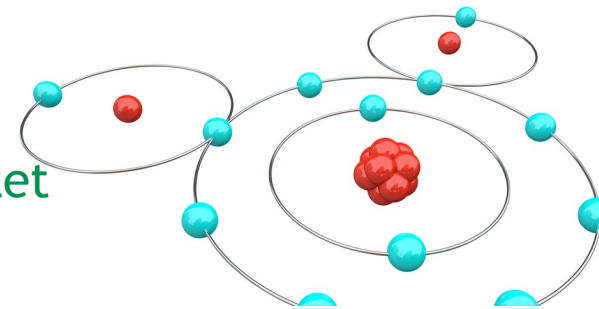
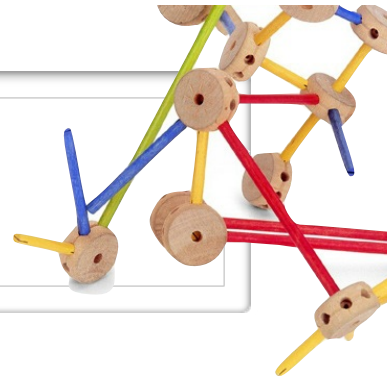




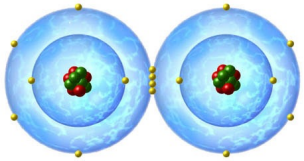


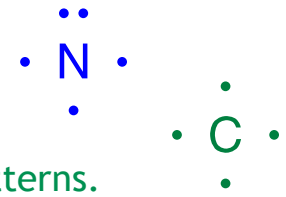
Ch06

Molecules

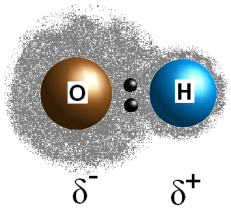


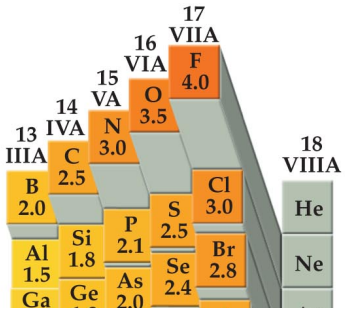
- Understanding Molecules
  - The covalent bond.
    - Gilbert Lewis
    - Connectivity
  - Lewis Notation
    - Lewis Symbols
    - The octet rule.
    - Explaining bonding patterns.





- Electronegativity
  - Polar covalent bonds
    - Bond Dipoles
  - Pauling values
    - Reference Values
    - ΔEN Thresholds
      - covalent, ΔEN = 0-0.4
      - polar covalent, ΔEN = 0.4-2.0
      - ionic, ΔEN = 2.0+





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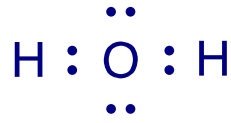

- Molecular Shape
  - Electron Pairs
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    - Electronic Structures
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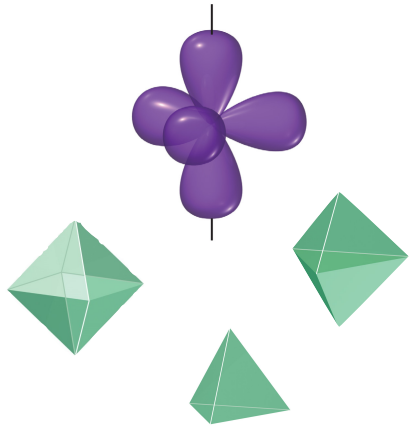

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  - Forces
    - Dipole-Dipole
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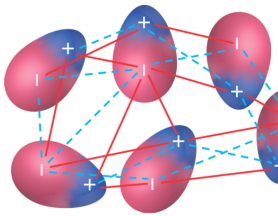
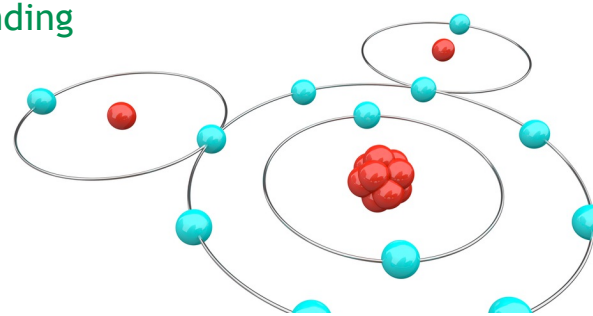
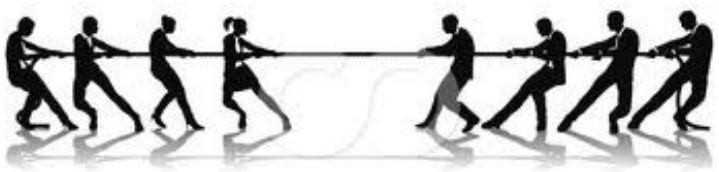
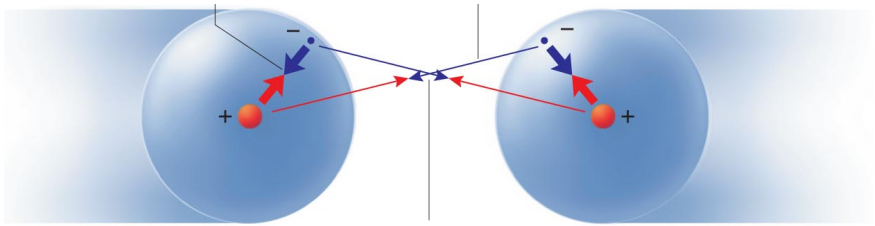
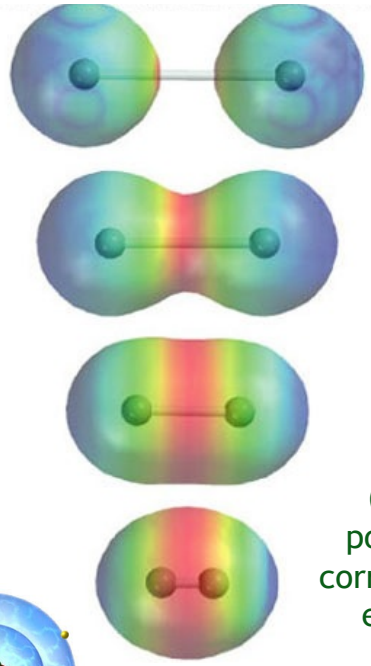


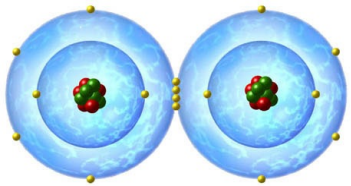


Covalent Bonds



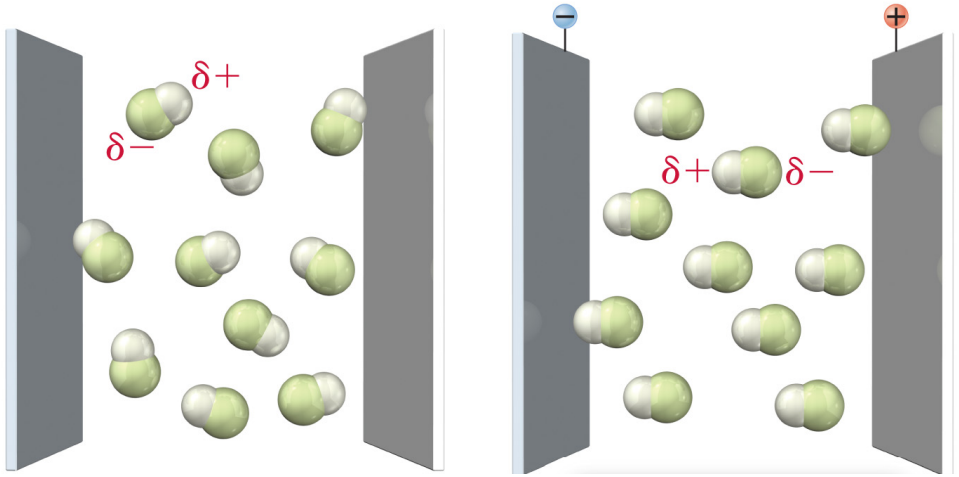




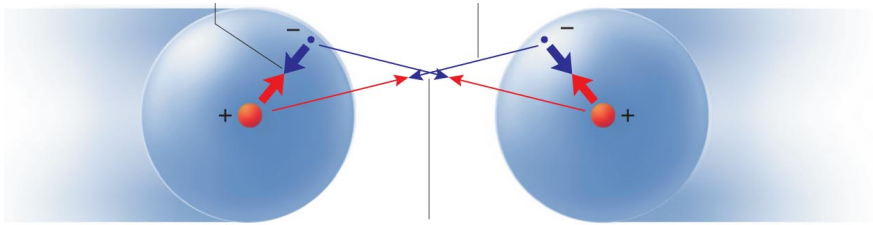


(in electrostatic potential maps red corresponds to greater electron density, blue indicates lesser density)

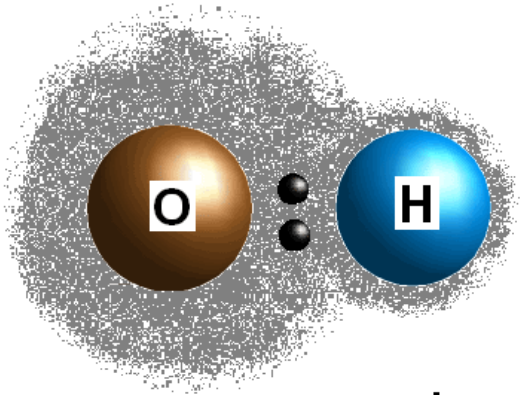
- Covalent Bonds are a result of atoms pulling on each others electrons.
- The atoms lock into a fixed distance from each other, entangling their orbitals.
- The shared electrons complete each atoms octet, making a stable combined arrangement of electrons.
- Some molecules placed in a electric field don't spin.
  - These molecules share electrons symmetrically, there is no positive of negative end to align with the field.
- Other molecules spin and align with the field.
  - These molecules must have a positive and negative end.
  - They don't share electrons symmetrically.

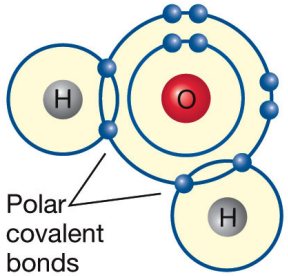


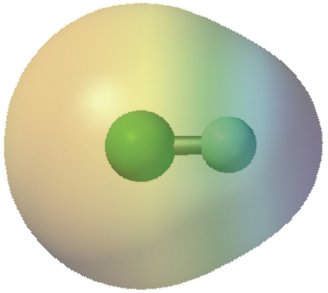
Polar Covalent Bonds

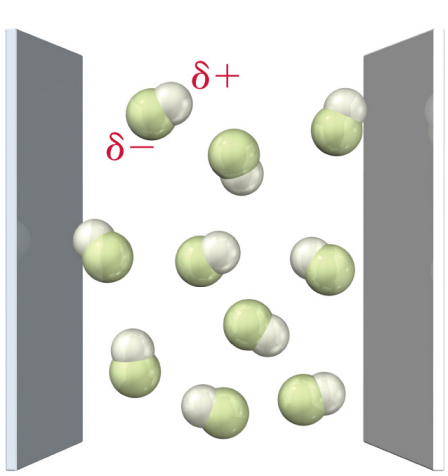


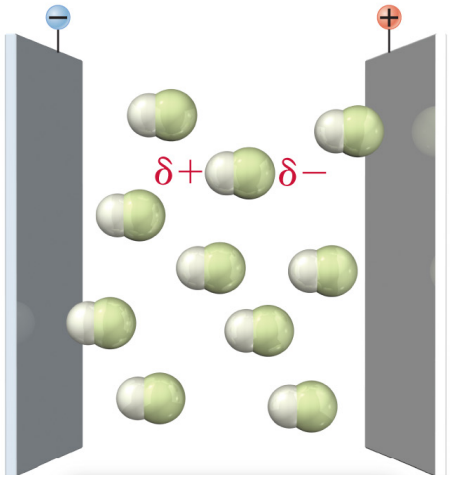
- Pure covalent bonds are symmetric.
  - Not all covalent bonds are pure.
- Sometimes one atom pulls stronger on the shared electrons than the other.
- Polar covalent bonds are covalent bonds with asymmetric sharing of the bonding pair.









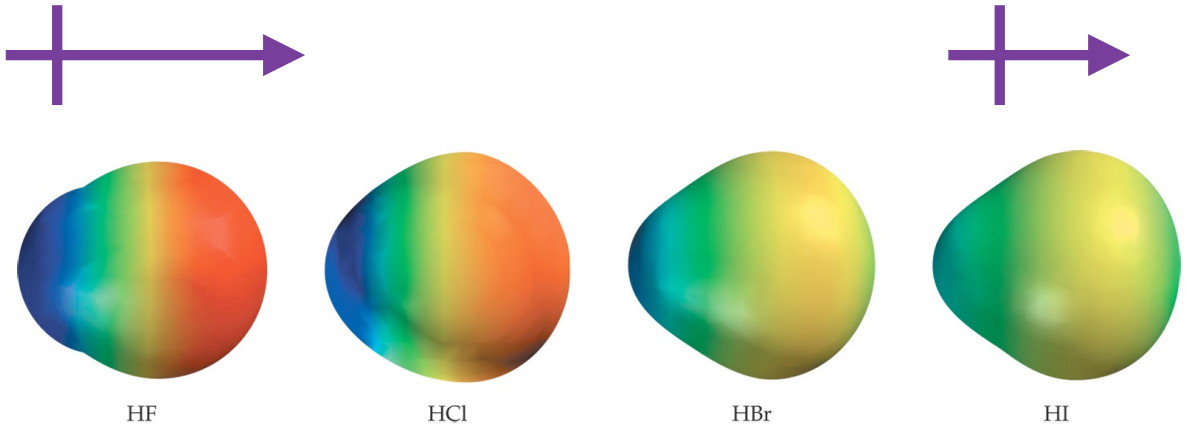


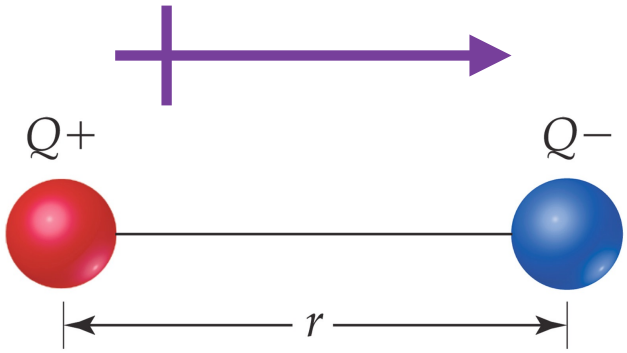
Bond Dipoles

- A separation of charge causes a dipole moment.
- The dipole moment, μ, produced by two equal but opposite charges separated by a distance, r, is calculated:

$$\mu = Qr$$

- Dipoles are measured in debyes (D).
- Q is measured in coulombs (C), r in meters (m).
- Dipoles are indicated graphically by an arrow pointing from the positive charge to the negative charge, with a cross on the positive end of the arrow.
- Polar covalent bonds have partial separation of charge, therefore have a dipole.
- The size of the dipole is indicated by the length of the arrow.
  - Longer arrows induce a larger dipole.
- To put numbers to polarity and dipoles we need a measure of the partial charge separation that occurs in polar covalent bonds.



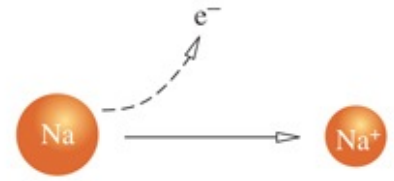


Electron Affinity (EA)

- Electron affinity is the energy released by adding an electron to an atom.
- Covalent bonding is a result of sharing electrons between atoms with high electron affinity.
- Less energy is released as we go down the periodic table.
- More energy is released as we go across the periodic table (left to right).
  - Noble Gases have a positive EA, no energy is released when they accept an electron.
    - They aren't very reactive.
  - Non-metals tend to have high EA, we get a lot of energy by giving them electrons.
    - Pure non-metals tend to be very reactive, they even react with themselves.
    - N_2, O_2, Cl_2, Br_2

Electron Affinities (kJ/mol)

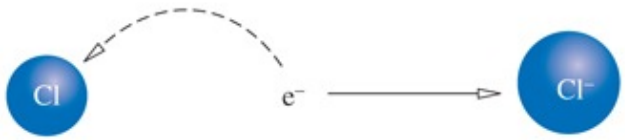
1A	2A	3A	4A	5A	6A	7A	8A
H −73							He >0
Li −60	Be >0	B −27	C −122	N >0	O −141	F −328	Ne >0
Na −53	Mg >0	Al −43	Si −134	P −72	S −200	Cl −349	Ar >0
K −48	Ca −2	Ga −30	Ge −119	As −78	Se −195	Br −325	Kr >0
Rb −47	Sr −5	In −30	Sn −107	Sb −103	Te −190	I −295	Xe >0



Ionization Energy (IE)

ΔH = +496 kJ/mol — endothermic

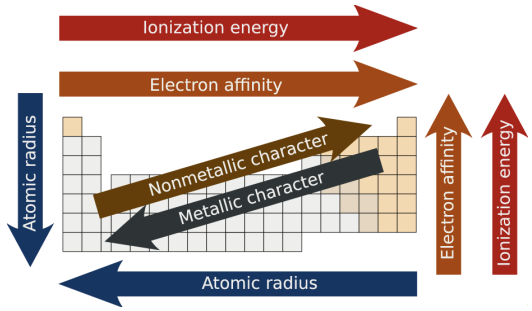
forming cations *consumes* energy



Electron Affinity (EA)

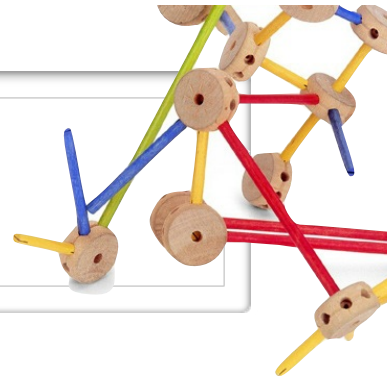
ΔH = -349 kJ/mol — exothermic

forming anions *releases* energy



Ch06

Molecules



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  - Polar covalent bonds
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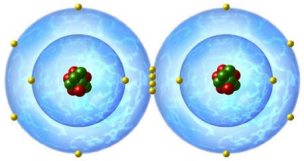
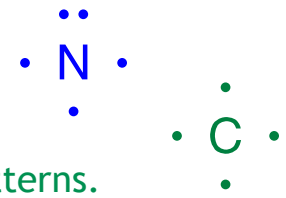
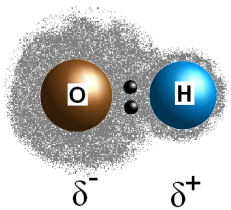
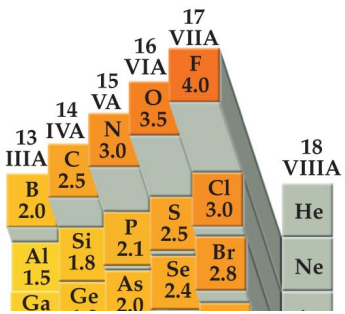


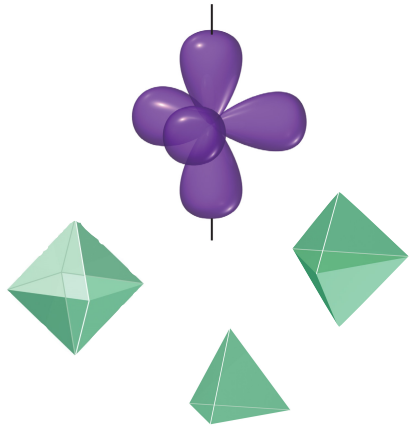






- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure



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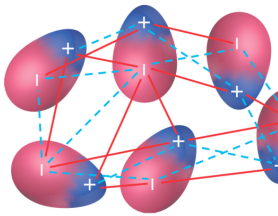
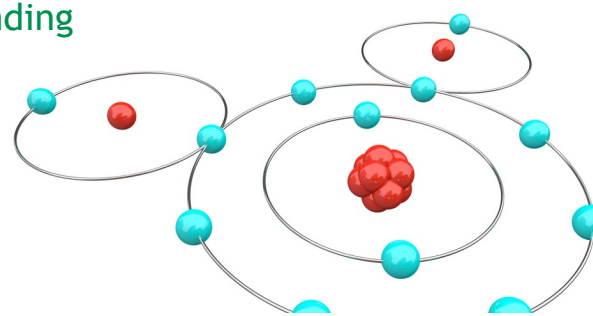
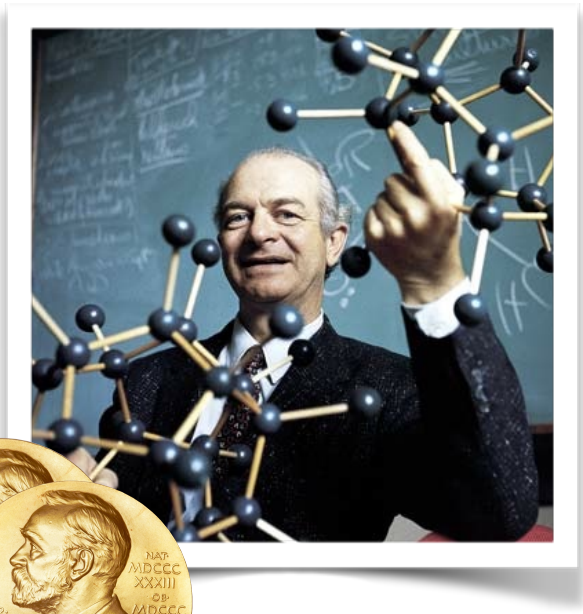
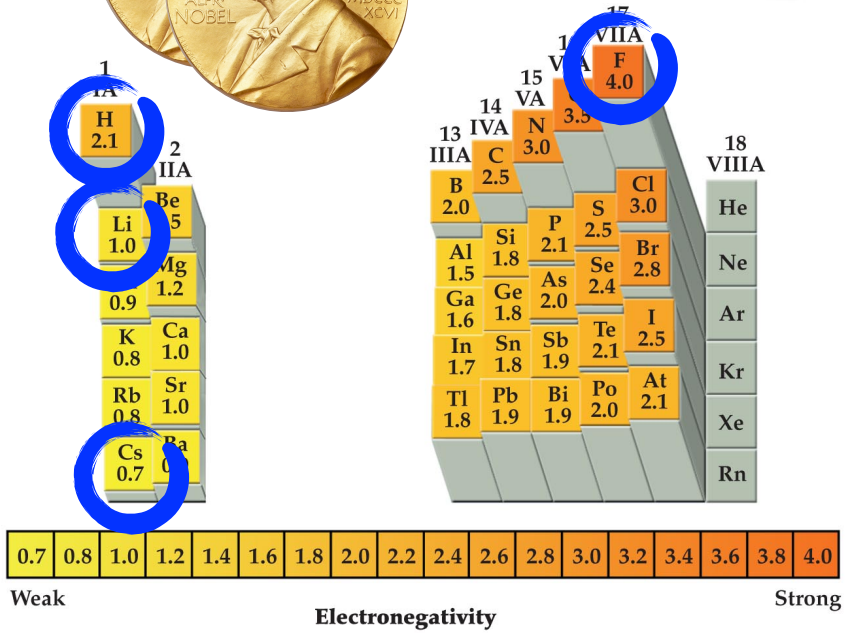




The Pauling Electronegativity Scale

- Electronegativity is a property of atoms within a molecule that is related to the electron affinity of that element.
- Electronegativity is the relative strength of an element pulling on electrons within the molecule.
- Unlike Electron Affinity and Ionization Energy…
  - Electronegativity is not measured in units of energy.
  - Electronegativity is not a threshold to forming ions.
- The electronegativity scale was established by CalTech professor Linus Pauling in 1932.
- Pauling was awarded the Nobel Prize in 1954 “for his research into the nature of the chemical bond” … and was also awarded the Nobel Peace Prize in 1962 for his work towards ending nuclear bomb testing.
- Linus Pauling is the only person to have every won two unshared Noble prizes.
- Electronegativity numbers are in Pauling units. Units are not shown.
- The electronegativity scale was established by looking at ratios of polar covalent bond strengths.
- You need to memorize four electronegativity values:
  - The values are based by the arbitrary assignment of 4.0 to Fluorine and 1.0 to Lithium.
    - As you go across the second period each element differs by 0.5.
  - Cesium has he lowest electronegativity of 0.7.
  - Hydrogen has a value of 2.1





Electronegativity Trends

- Electronegativity is the ability of atoms in a molecule to attract electrons to themselves.
- On the periodic chart, electronegativity increases as you go…
  - …from left to right across a row.
  - …from the bottom to the top of a column.
- Fluorine is the king.
- 2nd Period Elements differ by 0.5 each.

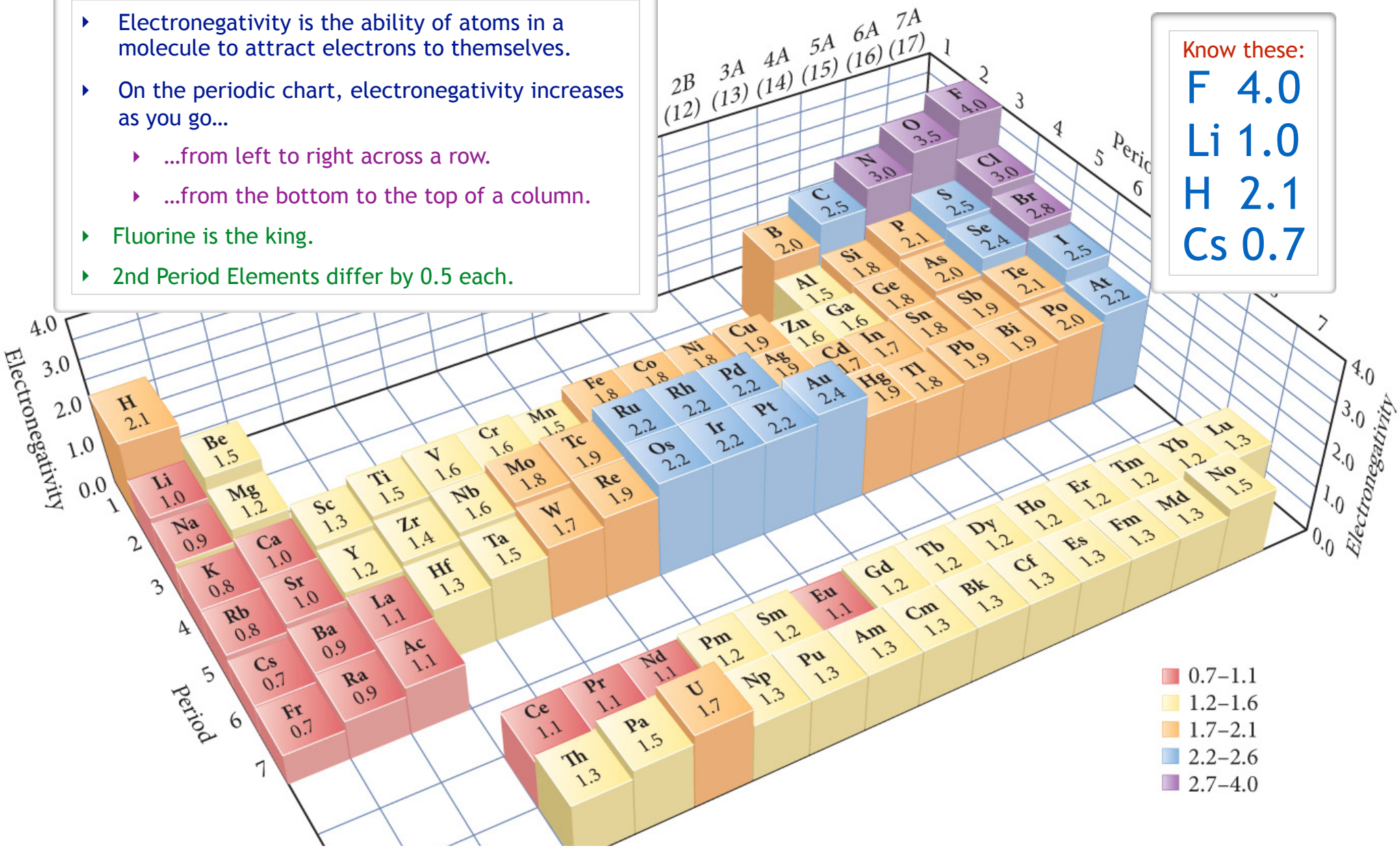
Know these:

F 4.0

Li 1.0

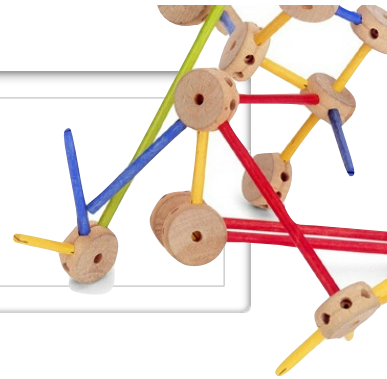
H 2.1

Cs 0.7



Ch06

Molecules



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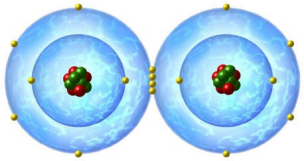

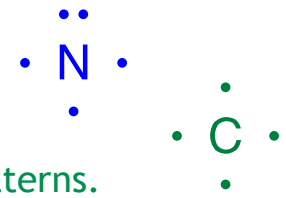

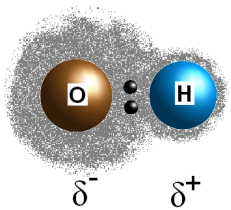

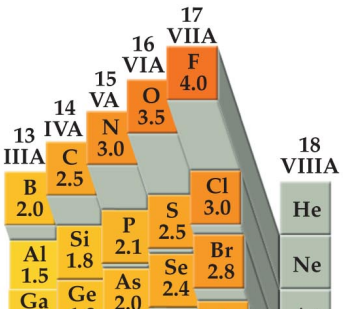

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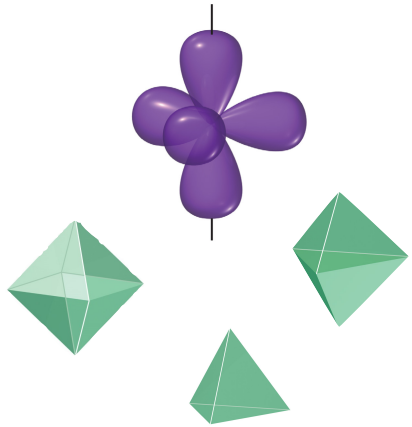
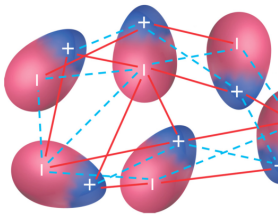
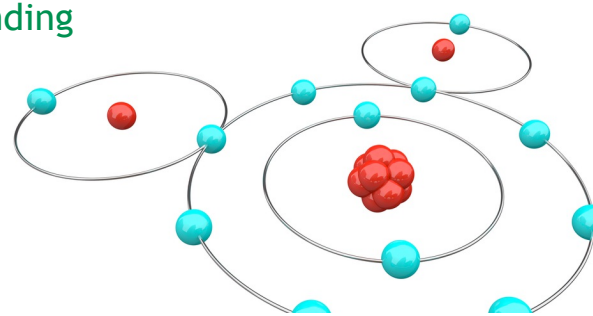
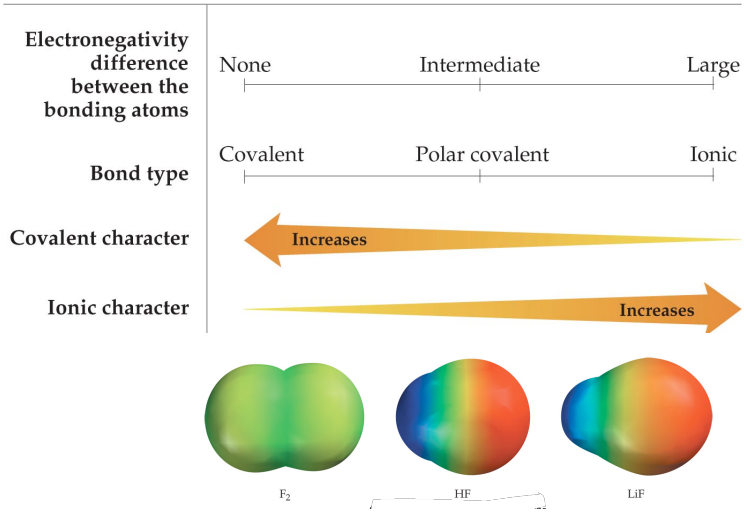






Identifying Bonding Types

- Lewis dot structures assume all bonds are covalent bonds.
- They're not.
- Bonding indicated by Lewis structures may turn out to be either:
  - Covalent (no dipole on the bond)
  - Polar Covalent (dipole along the bond)
  - Ionic (bond snaps and atoms become charged)
- Use the difference in electronegativity (ΔEN) to estimate the bond type.
  - The line between covalent & polar covalent is ΔEN = 0.4
  - The line between polar covalent & ionic is ΔEN = 2.0
    - Important: These lines are not exact, depending on the molecular structure there are many exceptions. But this is where we'll draw the lines for purposes of this class.

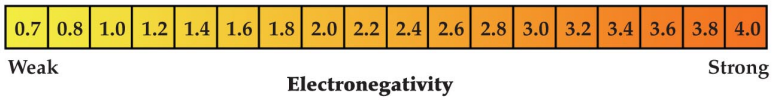


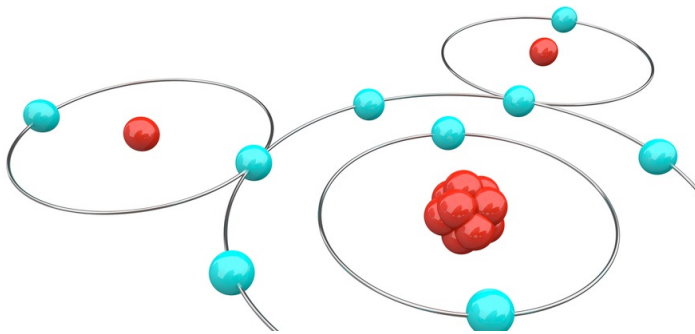
Bond	H—H	Cl—H	O—H	F—H
Electonegativity values of atoms	2.1 2.1	3.0 2.1	3.5 2.1	4.0 2.1
	2.1	3.0	3.5	4.0
	−2.1	−2.1	−2.1	−2.1
ΔEN	0	0.9	1.4	1.9
Type of bond	Covalent	Polar covalent		

Increasing polarity

H—H bond has a ΔEN of 0
(2.1 - 2.1 = 0) it's covalent.

Cl—H bond has a ΔEN of 0.9
(3.0 - 2.1 = 0.9) it's polar covalent.





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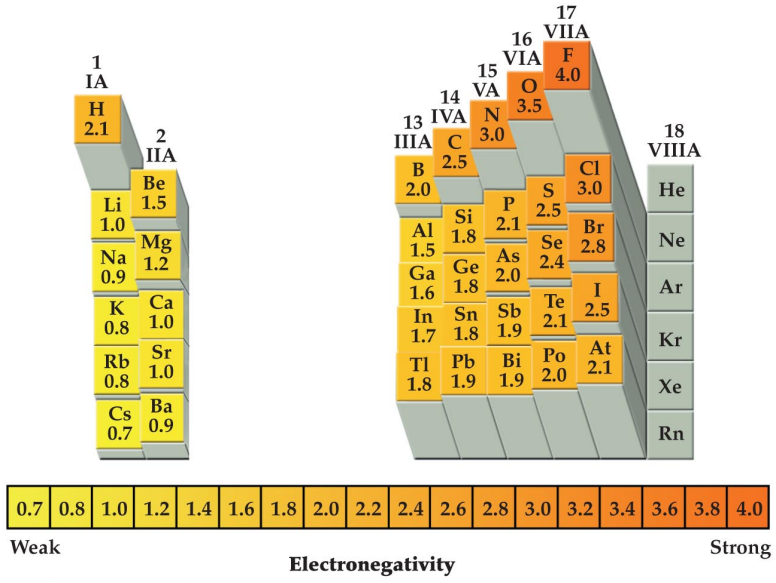
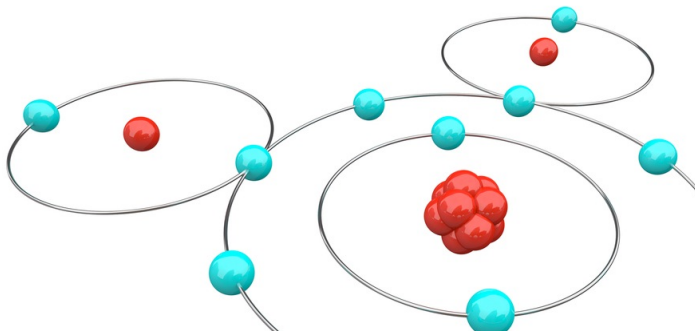


(PCl_3) P — Cl ΔEN = 0.9 Polar Covalent

(PH_5) P — H ΔEN = 0 Covalent

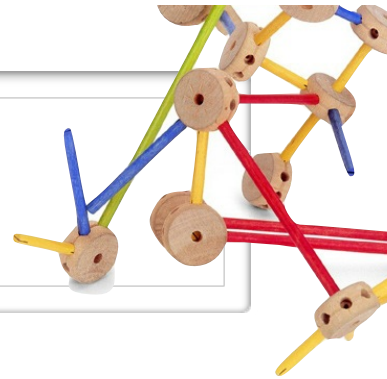
(Mg_3P_2) P — Mg ΔEN = 0.9 Polar Covalent

(MgO) O^{2-} Mg^{2+} ΔEN = 2.3 Ionic



Ch06

Molecules



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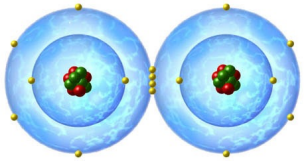
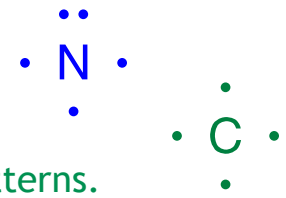
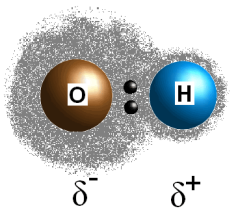
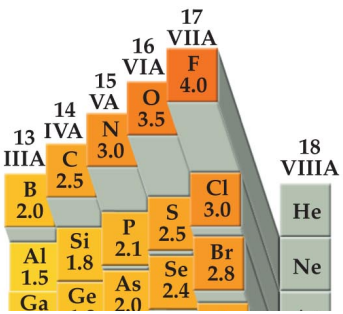
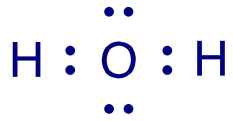




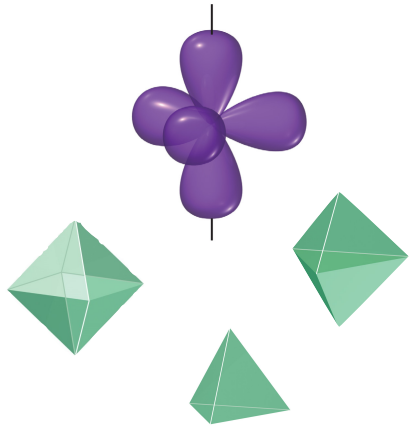




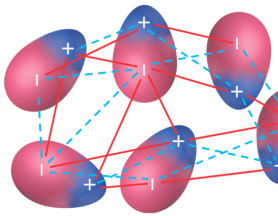
- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

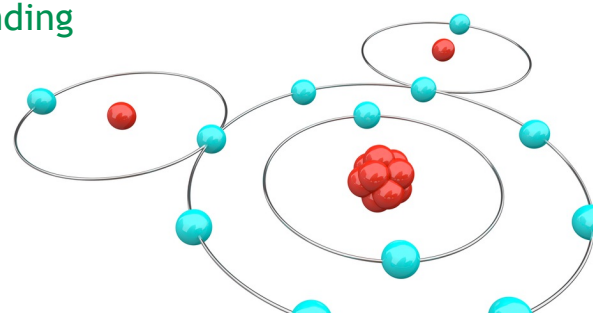


- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure



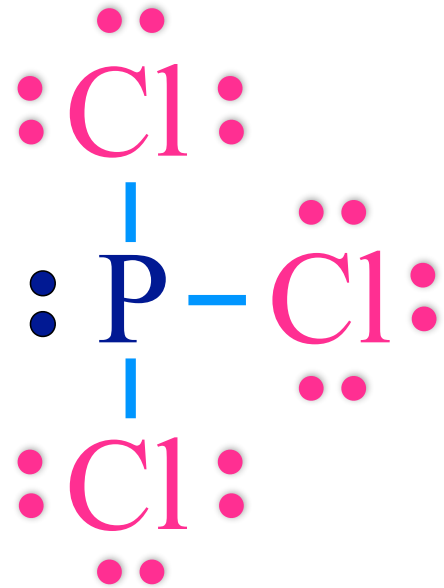
- Intermolecular Forces
  - Molecular Dipoles
  - Forces
    - Dipole-Dipole
    - London Forces
    - Hydrogen Bonding



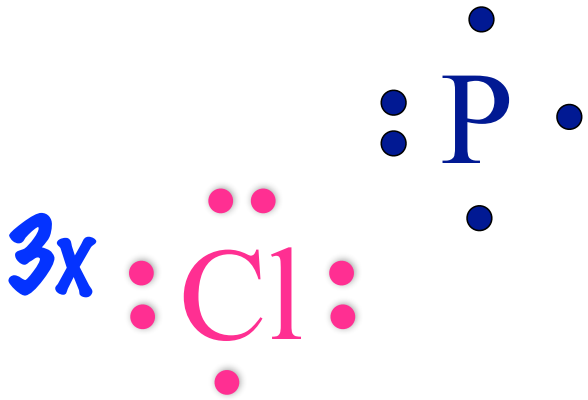


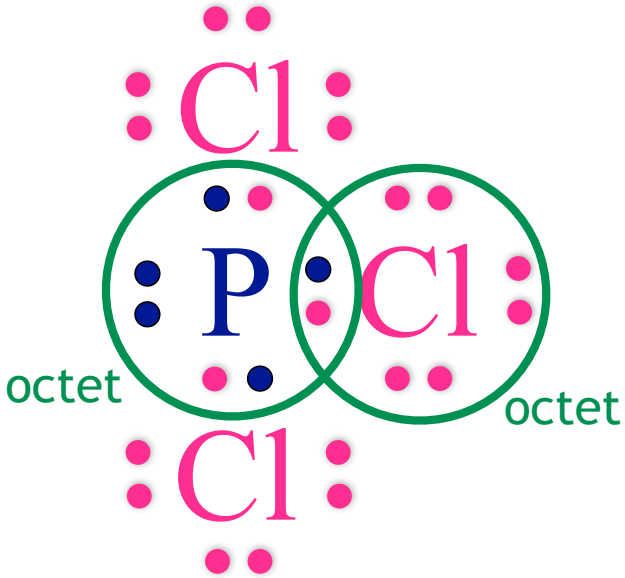
Lewis Structures

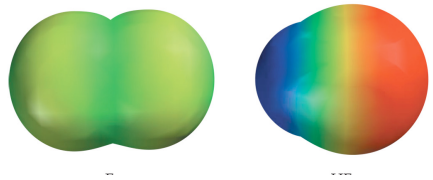
- A compound is formed by creating bonds between atoms.
- A compound is the result of atoms entangling their valence electrons, forming bonds.
- A Lewis structure is a description of a compound that shows where all the electrons of the atoms end up when the valence shells of the atoms entangle (form bonds).
- Good Lewis structures allow each atom to see an octet of electrons.
- A good Lewis structure is an accurate predictor of where bonds form in a compound.
- It helps us understand where bonds occur.
- Electrons group in pairs. Pairs are either shown as two dots or a single line.



PCl_3







How to make a Lewis Structure:

- Lewis structures are created by pooling all the electrons in a compound or ion and assigning them to bonds (shared electrons) and lone pairs (electrons dedicated to one atom).
- Use these five steps:
  - Step 1: Take Stock
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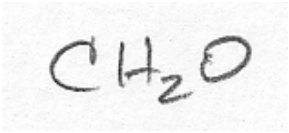
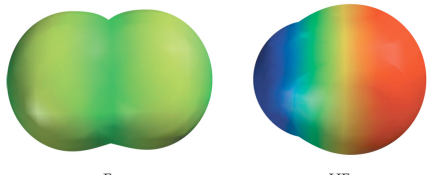
  - Step 4: Push LP's into Bonds
    - (if needed)
  - Step 5: Show any Charge





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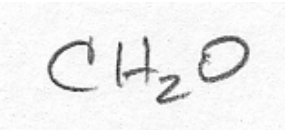

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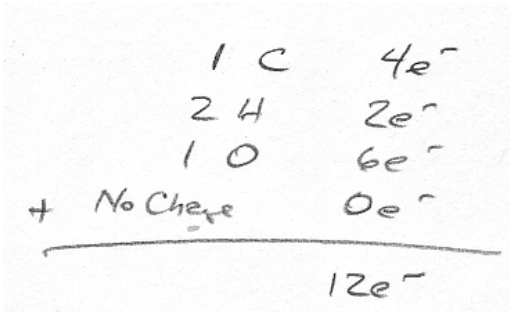

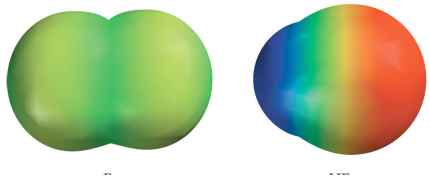

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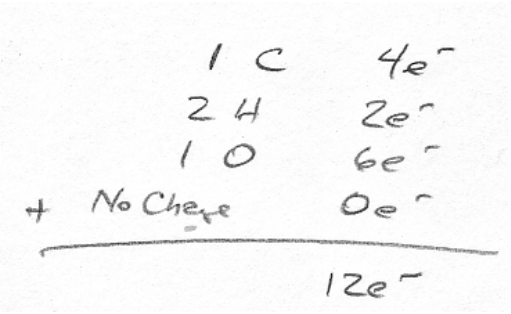

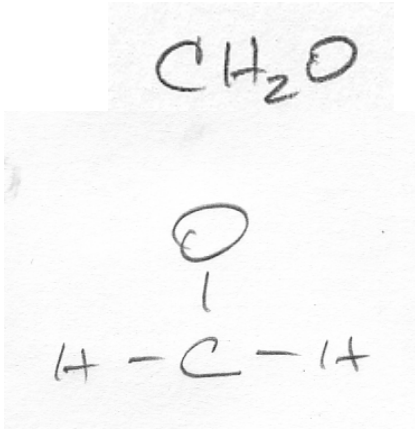

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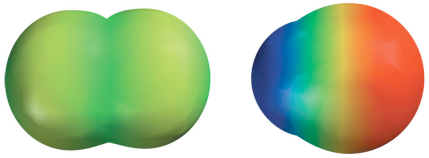

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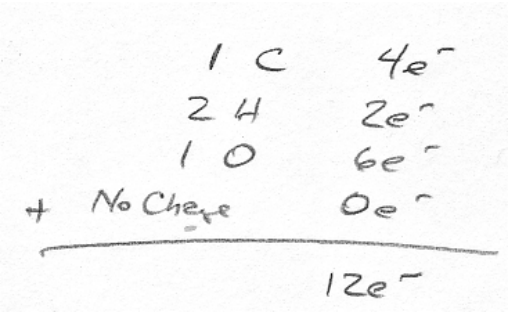
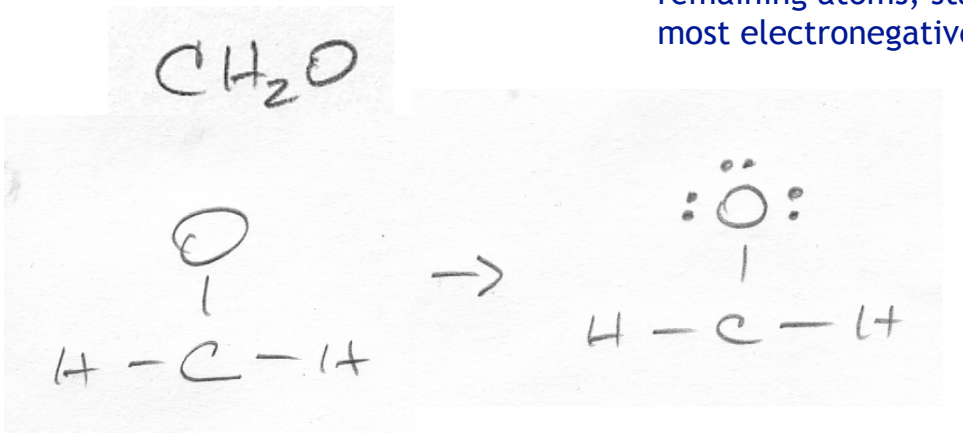
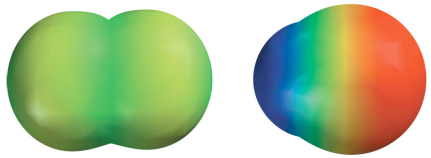
3. Fill in the Octets: Use the rest of the electrons to fill in the octets of remaining atoms, starting with the most electronegative atoms.







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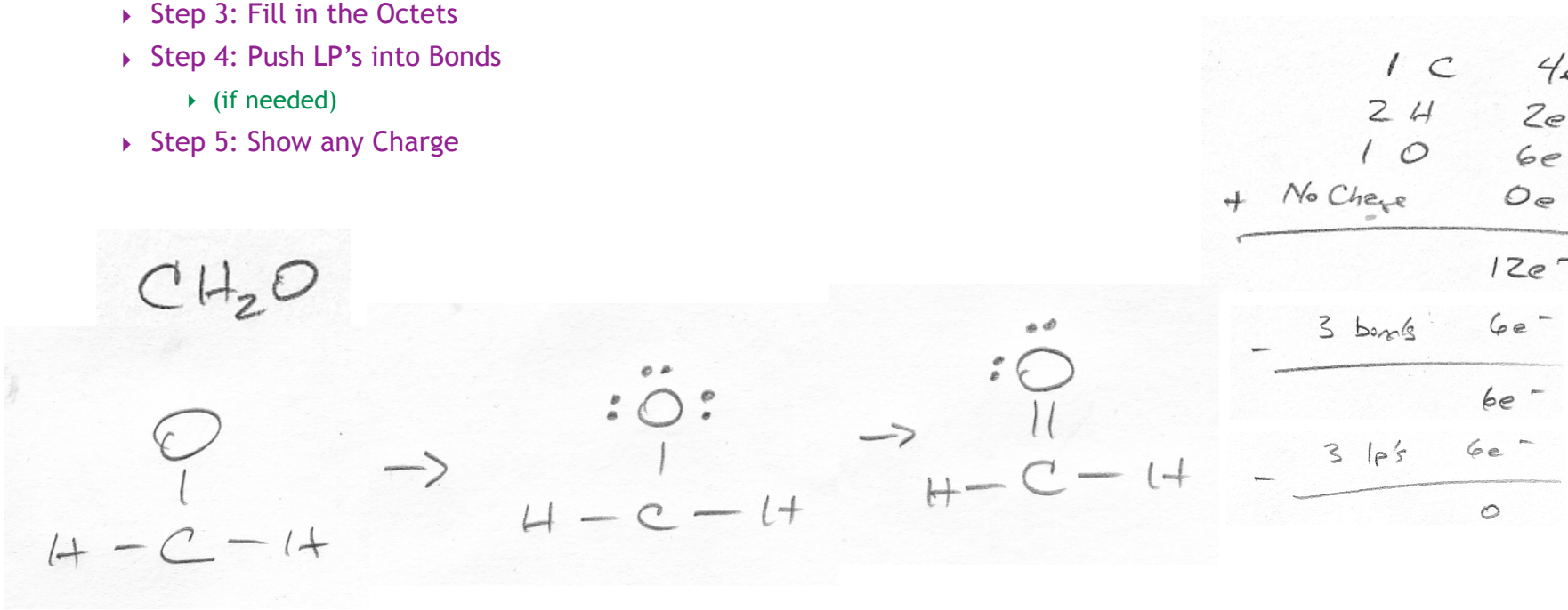
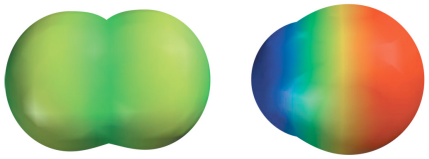


4. Push LP's into Bonds: If you run out of electrons before the central atom has an octets – form multiple bonds until it does.



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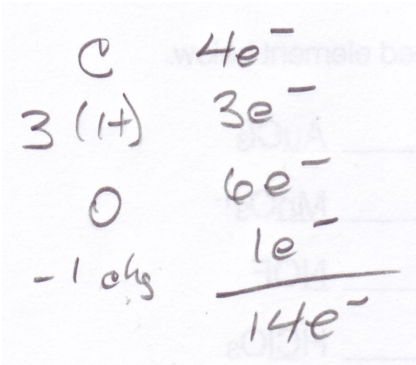

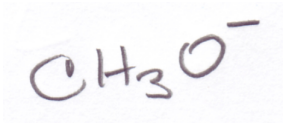

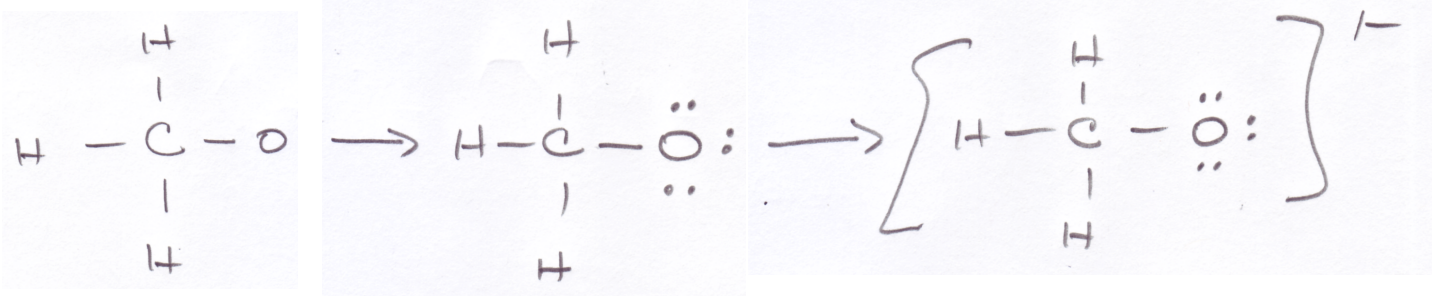

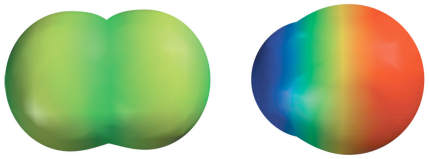

Try these…

- (1) Take Stock:
  - Find the sum of valence electrons of all atoms in the polyatomic ion or molecule.
    - If it is an anion, add one electron for each negative charge.
    - If it is a cation, subtract one electron for each positive charge.
- (2) Draw a skeleton:
  - The central atom is the least electronegative element that isn't hydrogen.
  - Look for chains or group hints in the formula.
  - Connect the atoms by single bonds (only).
- (3) Pass out the rest of the electrons:
  - Fill the octets of the outer atoms (most electronegative).
  - Fill the octet of the central atoms (least electronegative).
- (4) Push electrons:
  - If you run out of electrons before everyone has an octet…

    …form multiple bonds until they do.
- (5) Assign charge:
  - Show any overall charge.
  - Look at formal charge.
    - For each atom, count the electrons in lone pairs and half the electrons it shares with other atoms.
    - Subtract that from the number of valence electrons for that atom: the difference is its formal charge.

CO_2

CH_3OH

$CH_3CO_2^-$

NH_3

HCN

C_2H_4

NH_4^+

$CHOCH_3$

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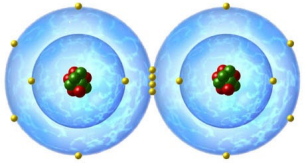
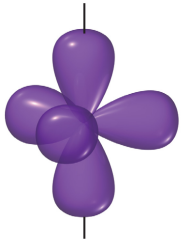
Ch06

Molecules

- Understanding Molecules
  - The covalent bond.
    - Gilbert Lewis
    - Connectivity
  - Lewis Notation
    - Lewis Symbols
    - The octet rule.
    - Explaining bonding patterns.
- Electronegativity
  - Polar covalent bonds
    - Bond Dipoles
  - Pauling values
    - Reference Values
    - ΔEN Thresholds
      - covalent, ΔEN = 0-0.4
      - polar covalent, ΔEN = 0.4-2.0
      - ionic, ΔEN = 2.0+





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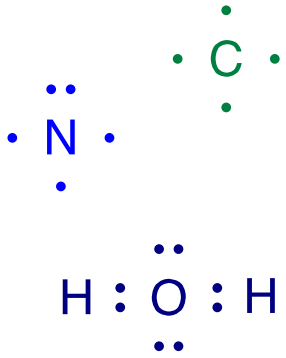
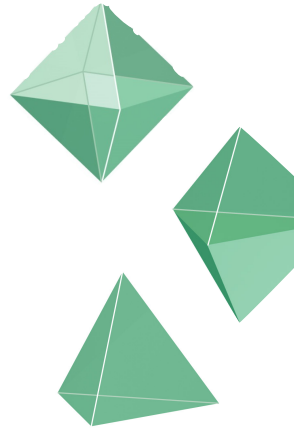
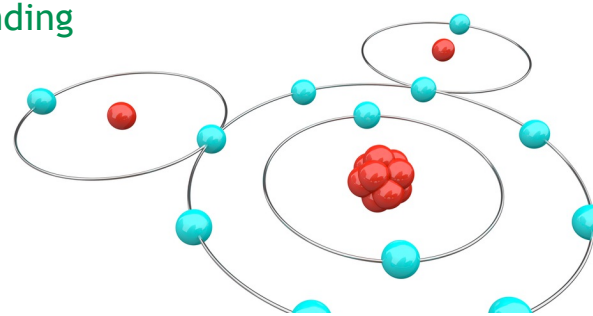


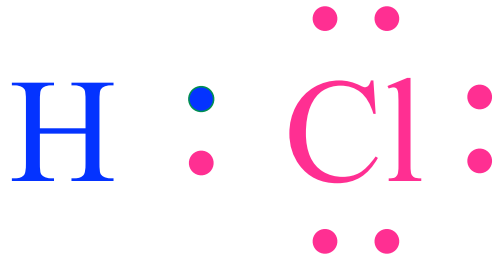




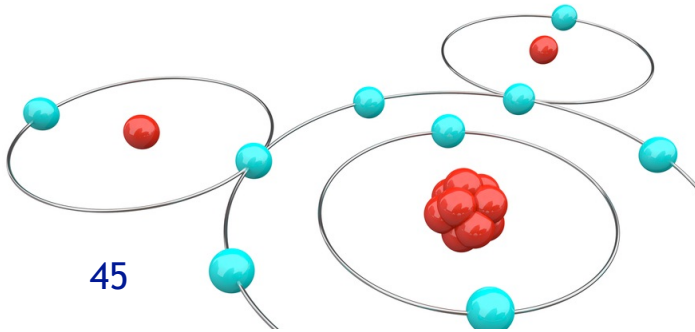
What Formal Charge is not.

- Formal Charge is not checking the octet.
  - When we build a Lewis structure, we try and make sure every atom is in a comfortable neighborhood.
  - Checking the octet is about finding out if atom sees the correct number of electrons around it.
  - This is not formal charge.
    - Chlorine has an octet, this has nothing to do with it's formal charge.
- Formal Charge is not oxidation number.
  - When we do redox chemistry, we ask ourselves what charge would an atom end up with if we broke every bond to create separate ions.
  - Chlorine normally has a -1 charge.
  - This is not formal charge.
    - It's oxidation number is -1, this has nothing to do with it's formal charge.
- Formal Charge is the formal "ownership" of electrons.
  - When we hypothesize a Lewis structure, we ask ourselves what price atoms paid to enter into that cooperative arrangement.
  - We ask ourselves how many electrons it ended up owning, and how many did it start with.
    - The difference is formal charge.
      - (# electrons in lone pairs + ½ in each of it's bonds - valence electrons for it's neutral atom)
    - Note: Any gains for one atom must be paid by another, so the sum of all formal charges must equal the total charge on the molecule or ion.
  - The higher the price, the less likely atoms will enter into that structure — formal charge let's us evaluate possible Lewis structures.

HCl



Valence	2e (duet)	8e (octet)
Oxidation Number:	+1	-1
Formal Charge:	0	0



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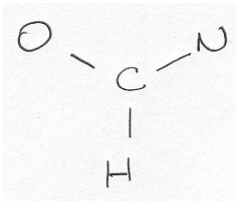
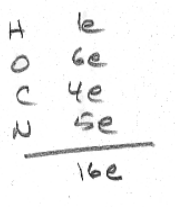
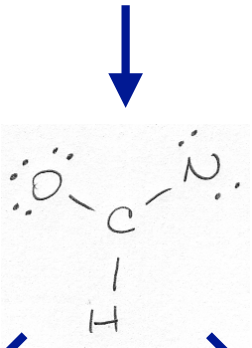
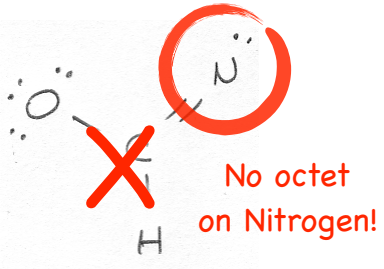
- Formal charge can be used to identify the "best" Lewis structure.
  - The best structure satisfies each atoms octet.
  - The best structure has a minimum of separation of charge.
  - The best structure places formal negative charge on the most electronegative elements.
  - The best structure places formal positive charge on the most electropositive elements.

HOCN

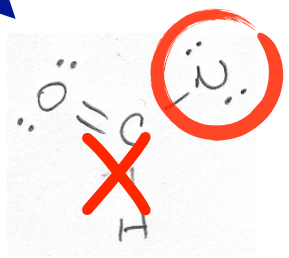








No octet on Nitrogen!



No octet on Nitrogen!

Neither structure is good. Start over.

Formal Charge

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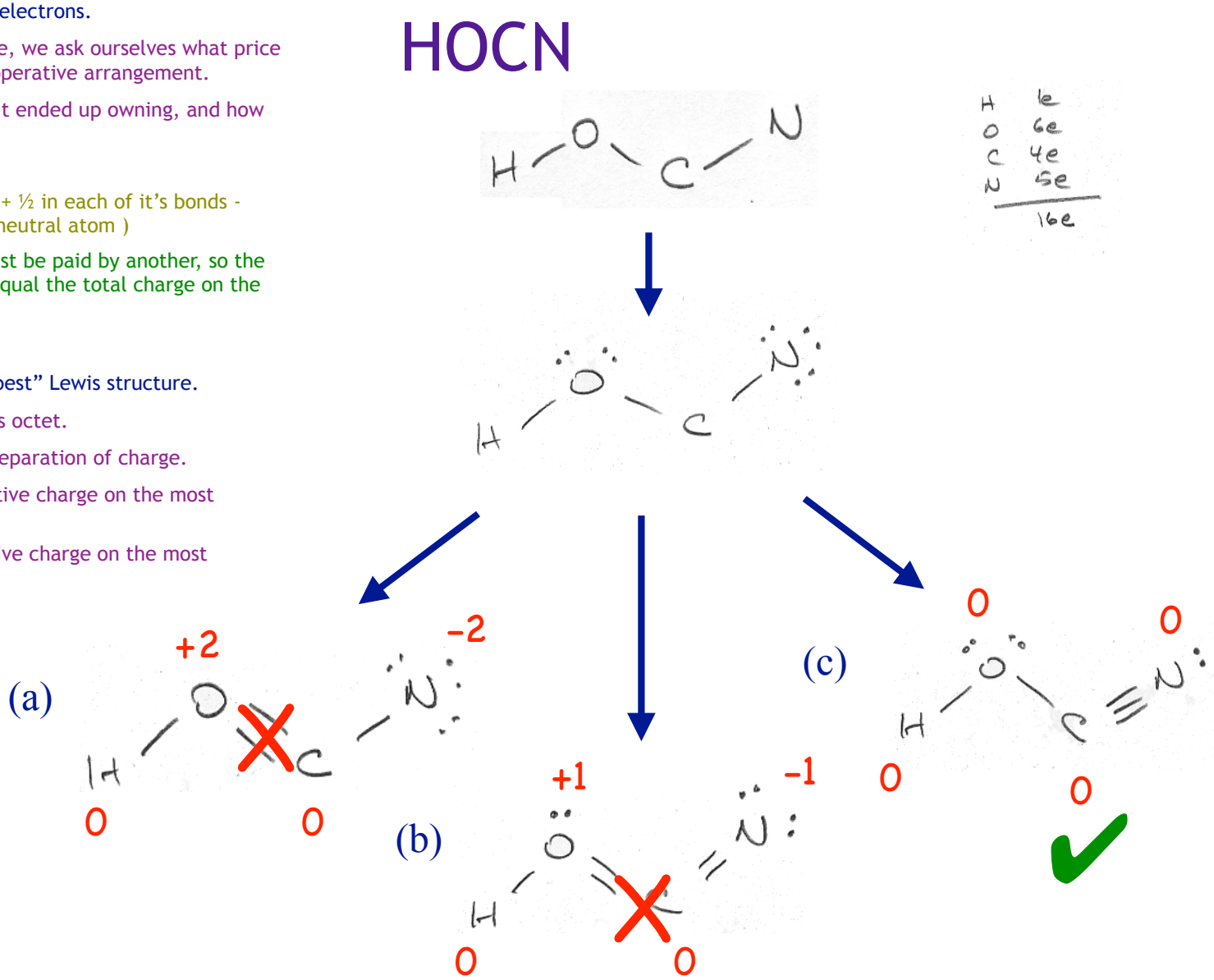
  - When we hypothesize a Lewis structure, we ask ourselves what price atom had to pay to enter into that cooperative arrangement.
  - We ask ourselves how many electrons it ended up owning, and how many did it start with.
    - The difference is formal charge.
      - (# electrons in lone pairs + ½ in each of it's bonds - valence electrons for it's neutral atom)
    - Note: Any gains for one atom must be paid by another, so the sum of all formal charges must equal the total charge on the molecule or ion.

- Formal charge can be used to identify the "best" Lewis structure.
  - The best structure satisfies each atoms octet.
  - The best structure has a minimum of separation of charge.
  - The best structure places formal negative charge on the most electronegative elements.
  - The best structure places formal positive charge on the most electropositive elements.



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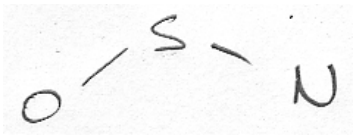
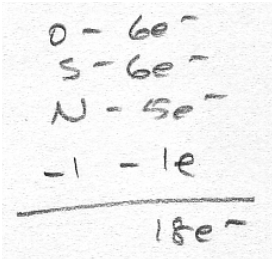
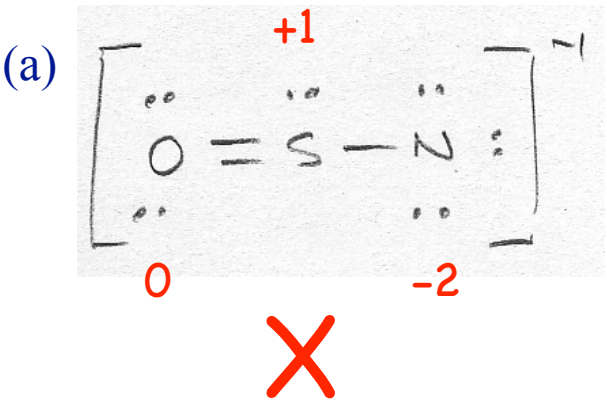
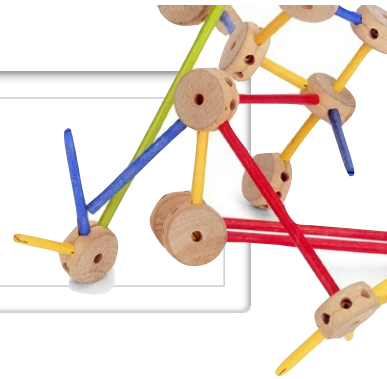






Ch06

Molecules



- Understanding Molecules
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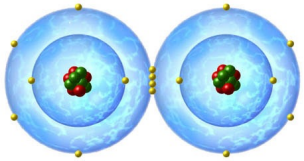
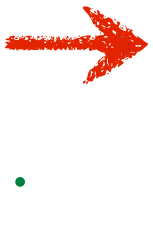
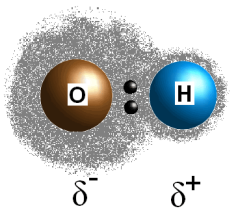
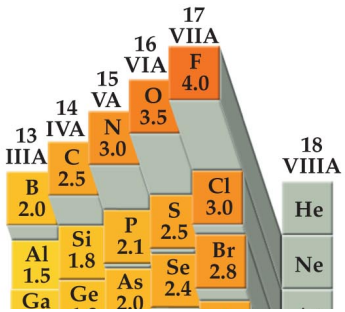


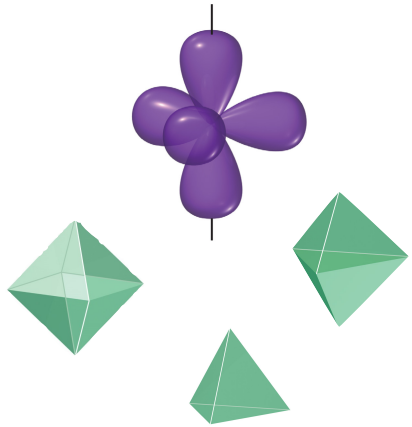






- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure



- Intermolecular Forces
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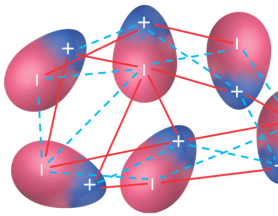
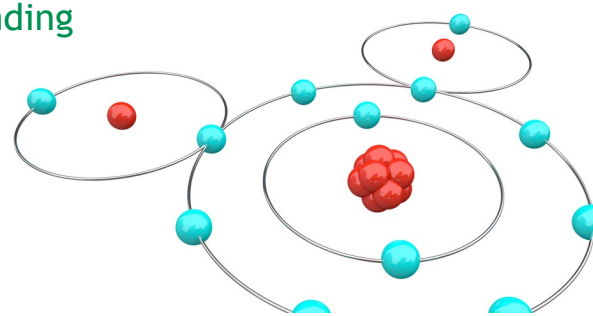




A model for predicting shape.

Composition

(What's in it.)

CCl_4

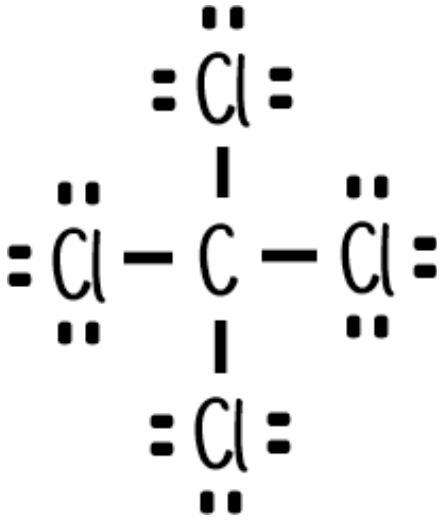
1 Carbon
4 Chlorine

Chemical Symbols

Molecular Formula

Connectivity

(What's connected to what.)

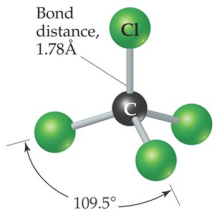


Lewis Dot Structure

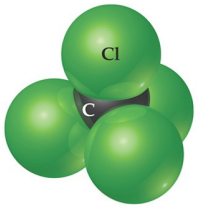
Shape

(Bond Angles & Distances)

(a)



(b)



(c)

VSEPR

Molecular Shape

- Properties of molecular substances depend on the structure of the molecule.
- The structure includes many factors:
  - The atoms that make up the molecule (composition).
  - The skeletal arrangement of the atoms and the kind of bonding between the atoms (connectivity).
    - Ionic, polar covalent, or covalent
  - The 3D form of the molecule (shape).
- Bonding theory should allow you to predict the shapes of molecules.
- Molecules are three-dimensional objects.
- We often describe the shape of a molecule with terms that relate to geometric figures.
- These geometric figures have characteristic “corners” that indicate the positions of the surrounding atoms around a central atom in the center of the geometric figure.
- The geometric figures also have characteristic angles that we call bond angles.
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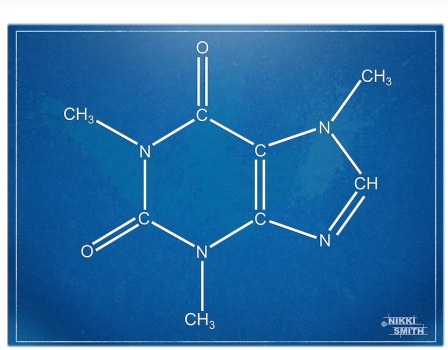
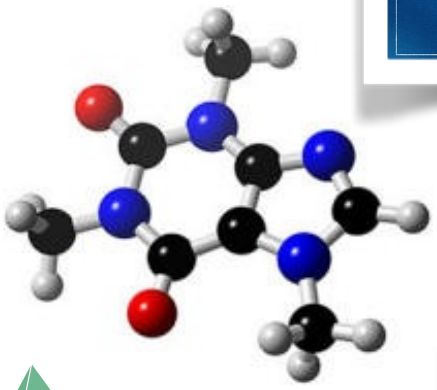
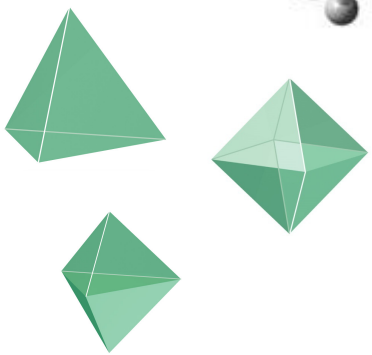
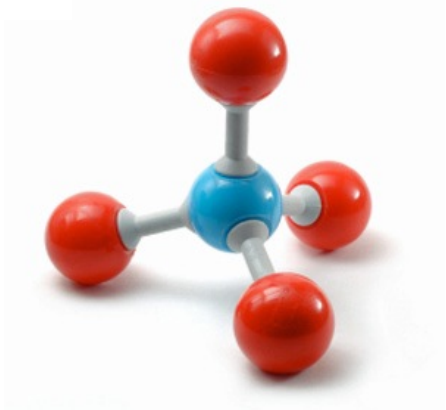
$C_8H_{10}N_4O_2$



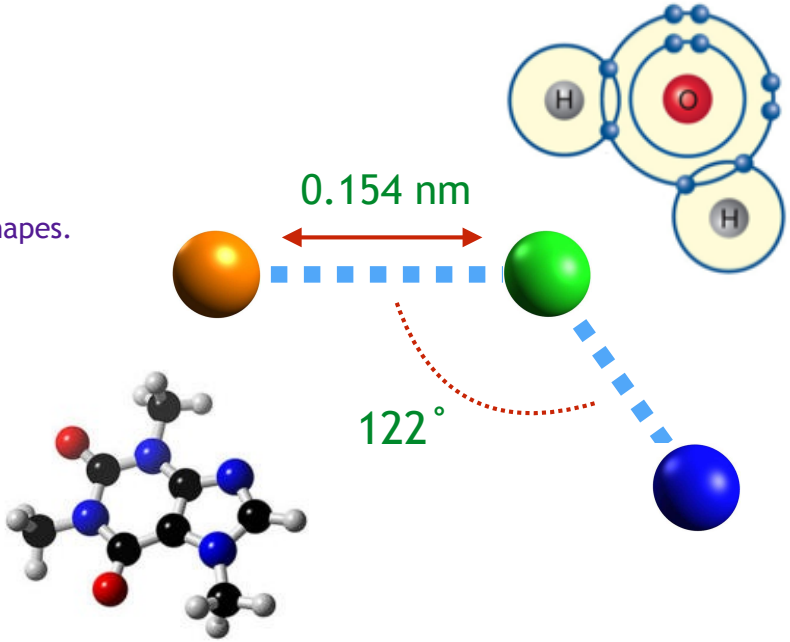




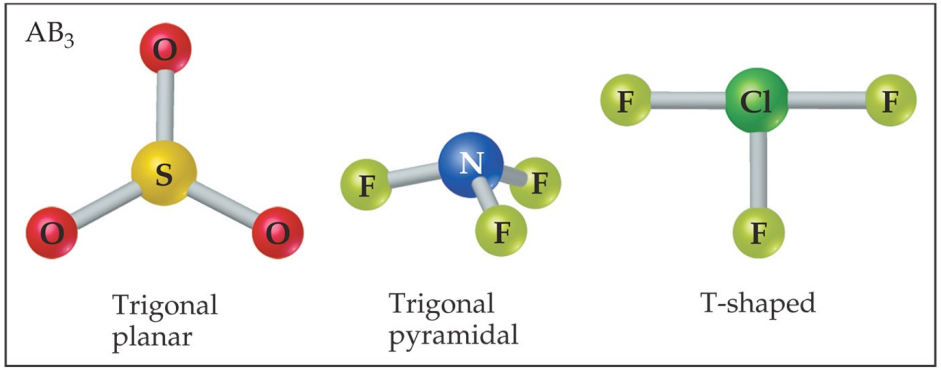


Defining Molecular Shape

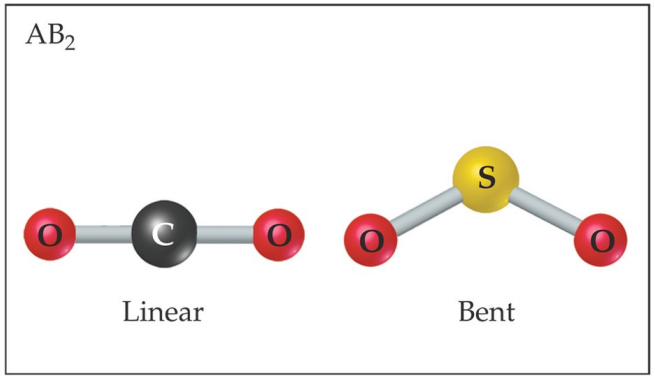
- Covalent bonds lock electrons into positions between atoms.
- Multiple covalent bonds can connect to a central atom in different geometries.
- Geometries are defined by:
  - bond angles: the angle between two bonds
  - bond distances: the distance between two bonded atoms
- Molecules can have the same composition, same connectivity — but different shapes.
  - A central atom with two valence atoms can be:
    - Bent
    - Linear
  - A central atom with three valence atoms can be:
    - Planar
    - Pyramidal
    - T-Shaped
- Overall molecular shape is the sum of shape around each atom.
- The shape of a molecule plays an important role in its reactivity.
- We need a tool to predict valence atom shapes.



3 Valence Atom Shapes

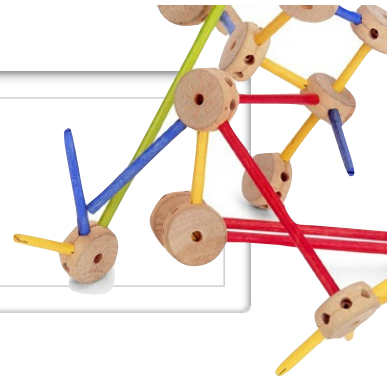


2 Valence Atom Shapes



Ch06

Molecules



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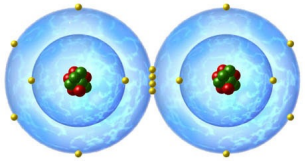

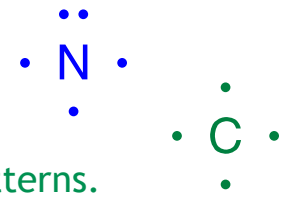

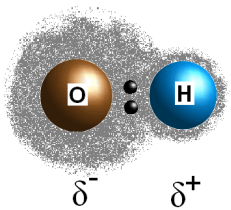

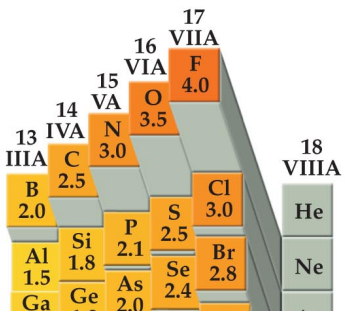

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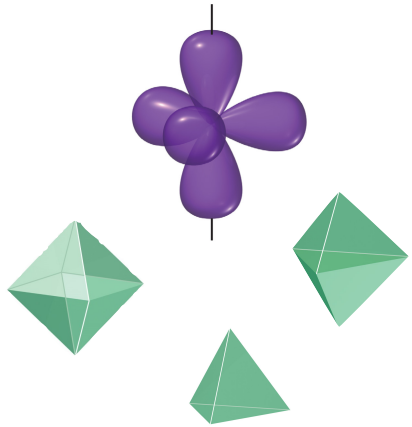

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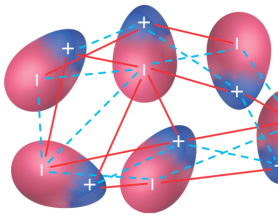
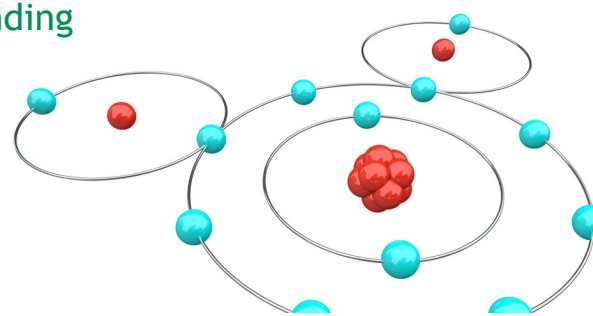
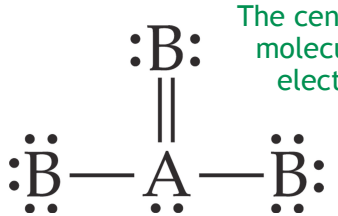


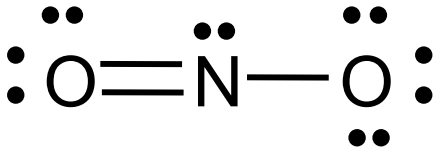


Electron Domains

- To identify the shape around atoms in a molecule, we need to understand the shape formed by the electron pairs around that atom.
- By noting the number of bonding and nonbonding electron pairs we can predict bond angles and distances.
- We refer to the electron pairs as electron domains.
  - In a double or triple bond, all electrons shared between those two atoms are on the same side of the central atom; therefore, they count as one electron domain.
- This allows us to predict the shape of a molecule, by considering electron repulsion…

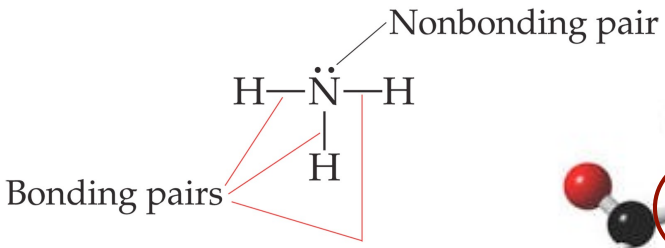


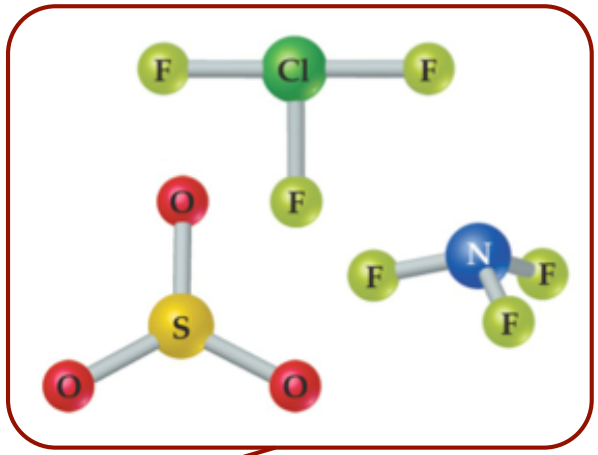
The central atom in this molecule, A, has four electron domains.

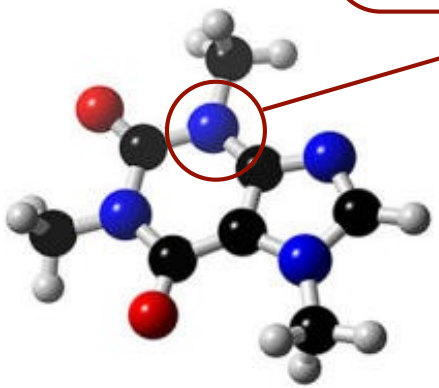


There are three electron groups on N:

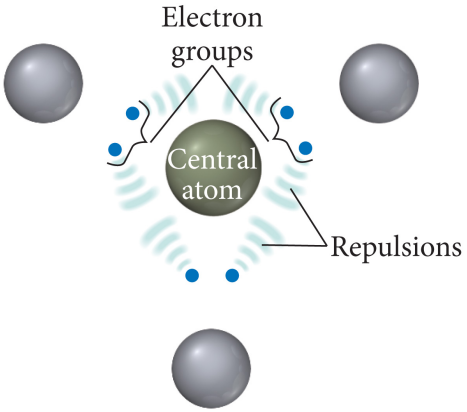
- One lone pair
- One single bond
- One double bond







Electron Repulsion

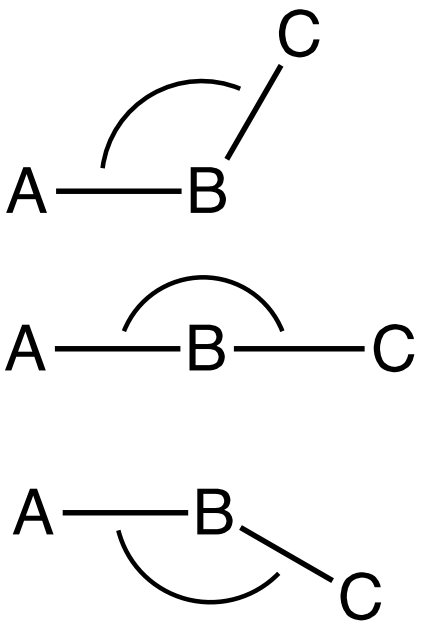


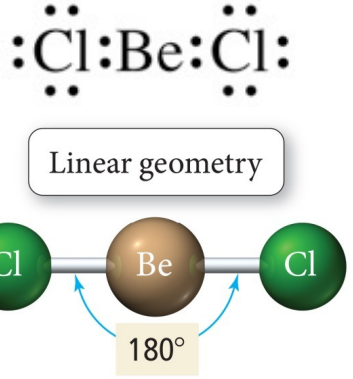
- Electron pairs, whether they be bonding or nonbonding, repel each other.
- By assuming the electron pairs are placed as far as possible from each other, we can predict the shape of the molecule.
- There are five basic arrangements of electron groups around a central atom.
  - That's based on a maximum of six bonding electron groups around an atom.

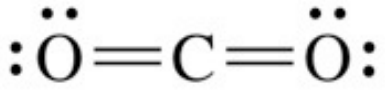
    (There may be more than six on very large atoms, it is very rare. – We won't worry about those)
- Each of these five basic arrangements results in five different basic electron geometries.
  - In order for the molecular shape and bond angles to be a "perfect" geometric figure, all the electron groups must be bonds and all the bonds must be equivalent.
    - We'll tweak the model later to account for differences.
  - For molecules that exhibit resonance, it doesn't matter which resonance form you use as the underlying electron geometry will be the same.
- All atoms that have 2-6 Electron Domains will have their electron pairs arranged in one of these five basic geometries.

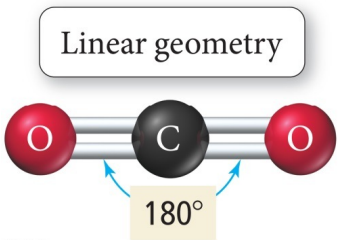
2 Electron Domains — Linear

- The best arrangement of two electron domains around a central atom is linear.
- A pushes C away until the ABC bond angle is 180˚
- Pushing any farther than 180˚ brings C closer to A — on the other side.



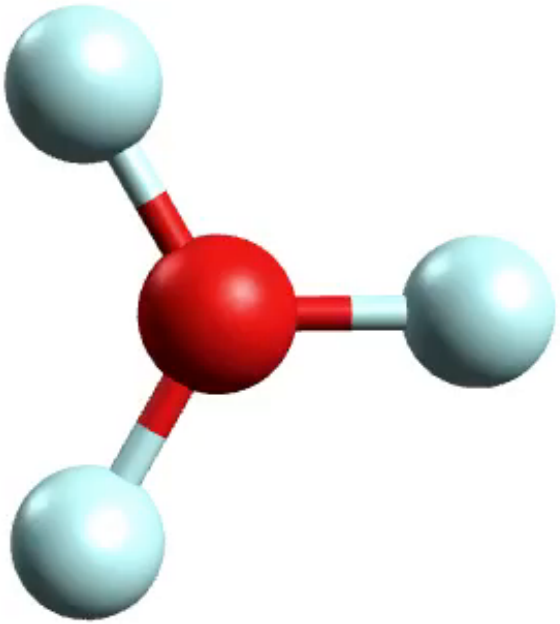


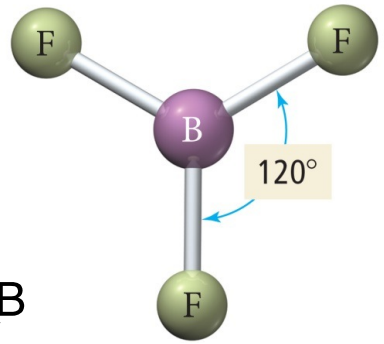


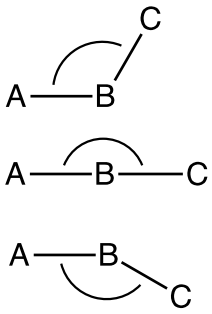


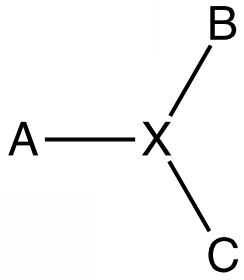
3 Electron Domains – Trigonal Planar

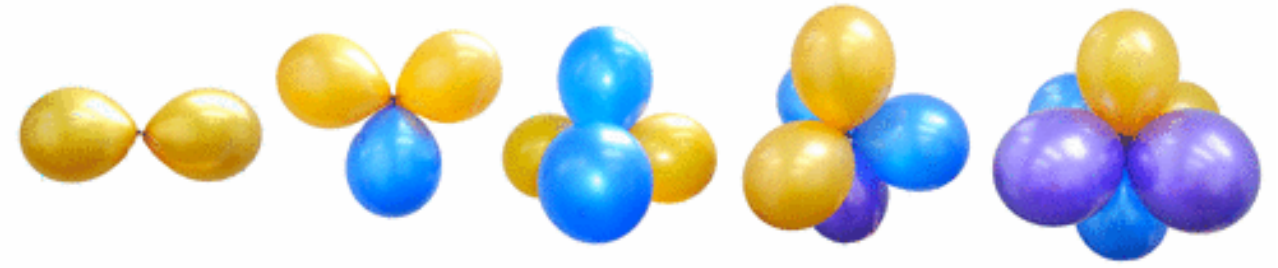
- Three electron domains around a central atom form a trigonal planar arrangement.
- The bond angle between each atom is 120˚
- The three domains remain in the same plane for the same reason they remain linear when there are two domains.

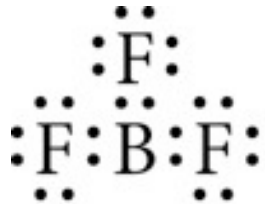






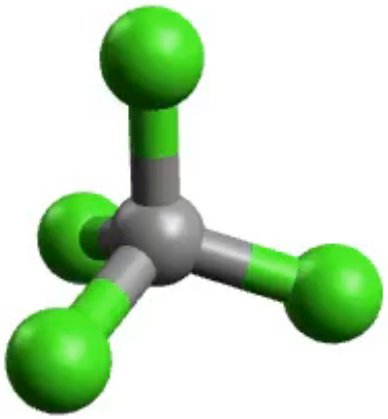


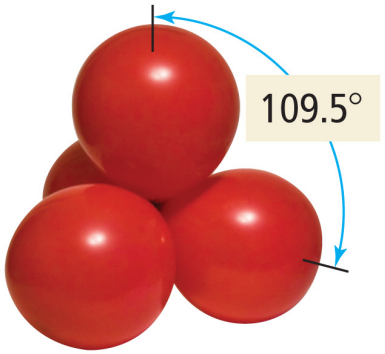


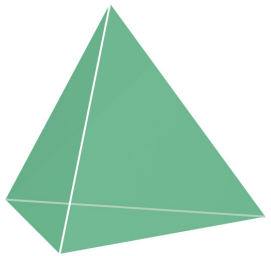


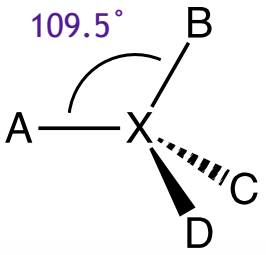
4 Electron Domains — Tetrahedral

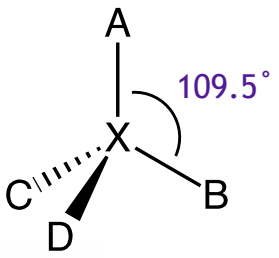
- Four electron domains form a tetrahedral arrangement around the central atom.
- A tetrahedron, a pyramid with a triangular base, defines the position of each domain.
- All domains are equidistant from each other.
- The bond angle between any two domains is 109.5˚
- To draw a tetrahedral atom, draw three atoms in the plane and then use a dotted line to show one behind and a triangle to show one in front.

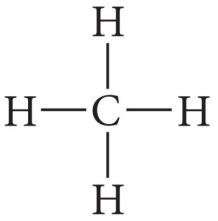


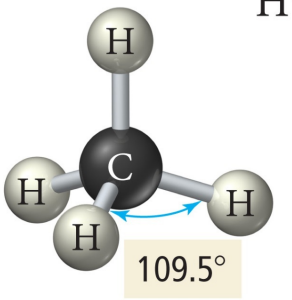






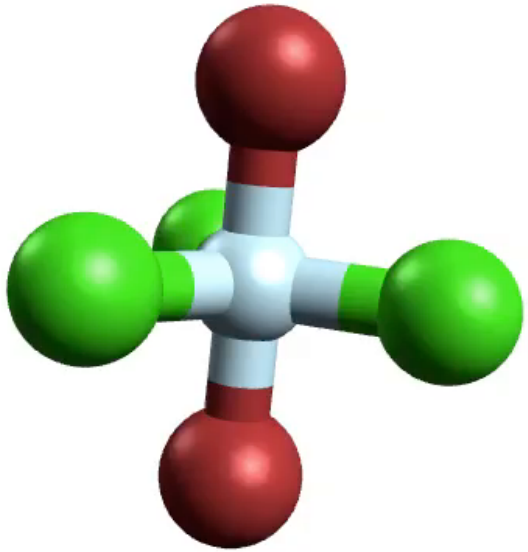


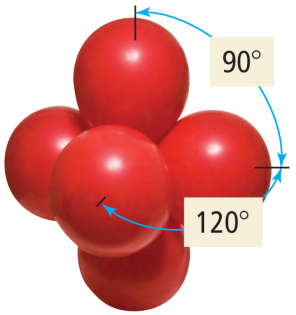


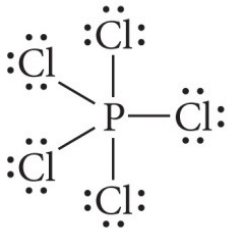


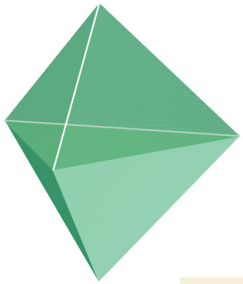
5 Electron Domains — Trigonal Bipyramidal

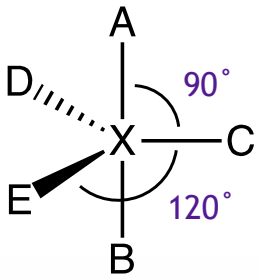
- Five electron domains form a trigonal bipyramidal arrangement around the central atom.
- This optimal arrangement has two types of positions:
  - Equatorial
  - Axial
- Equatorial positions are 120˚ apart.
- Axial positions are above and below the equatorial plane.
- Axial positions are 90˚ from the equatorial plane.

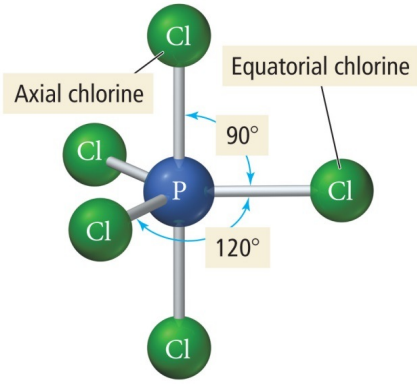








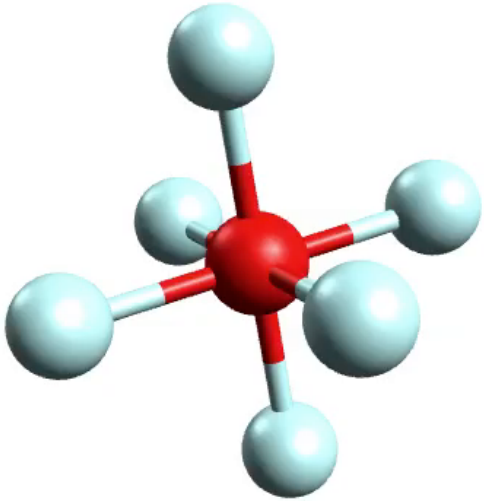


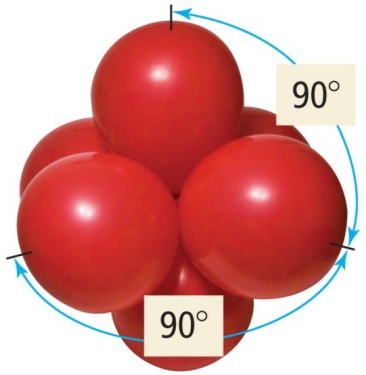


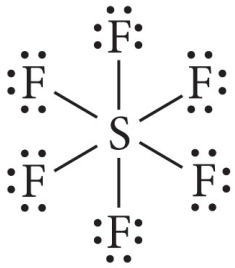
6 Electron Domains – Octahedral

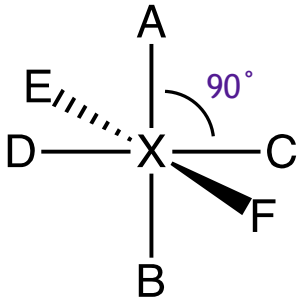
- Six electron domains form an octahedral arrangement around the central atom.
- The points of an octahedron geometric shape defines the positions of domains in an octahedral arrangement.

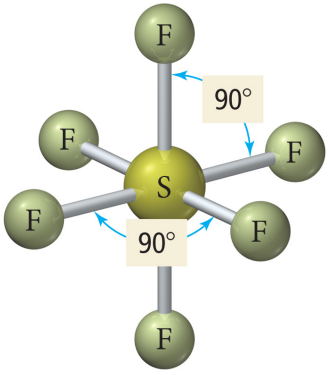
  (Played D&D? Think 8 sided dice!)
- All six positions are equivalent.
- Each position is equidistant from 4 other positions and forms a 90˚ angle with each.
- It is also opposite the last position and has 180˚ angle with it.











	Electronic Geometry	Bond Angles
1 e pair	Linear	180˚
2 e pair	Linear 	180˚
3 e pair	Trigonal Planar 	120˚
4 e pair	Tetrahedral 	109.5˚
5 e pair	Trigonal Bipyramidal 	90˚ and 120˚
6 e pair	Octahedral 	90˚

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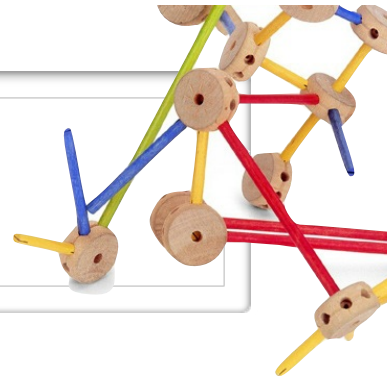
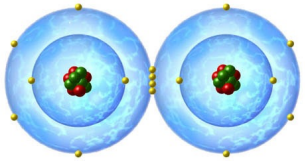
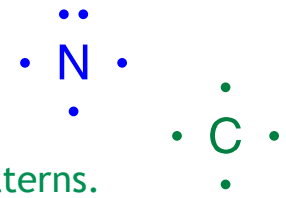
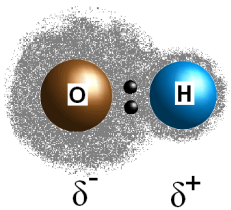
Molecules

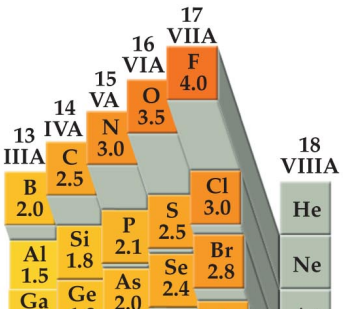


- Understanding Molecules
  - The covalent bond.
    - Gilbert Lewis
    - Connectivity
  - Lewis Notation
    - Lewis Symbols
    - The octet rule.
    - Explaining bonding patterns.
- Electronegativity
  - Polar covalent bonds
    - Bond Dipoles
  - Pauling values
    - Reference Values
    - ΔEN Thresholds
      - covalent, ΔEN = 0-0.4
      - polar covalent, ΔEN = 0.4-2.0
      - ionic, ΔEN = 2.0+



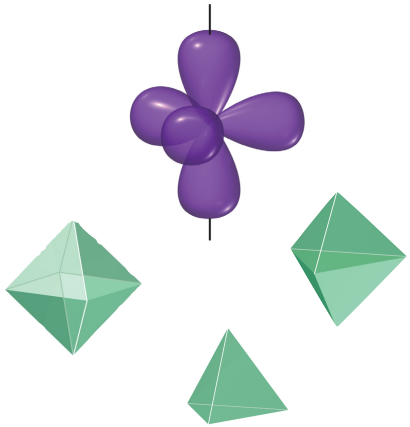


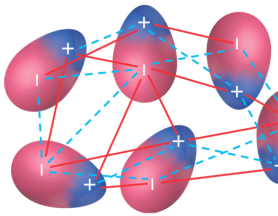


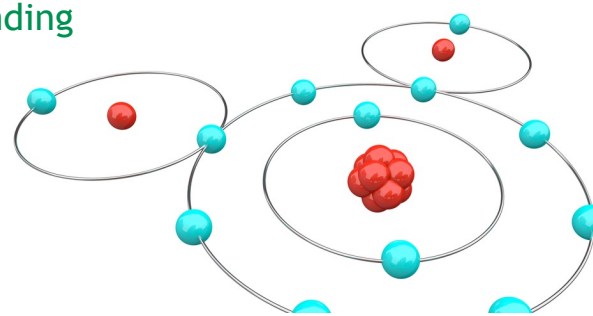


- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

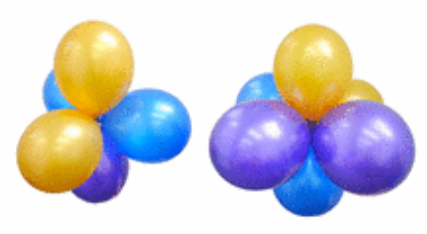
- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure
- Intermolecular Forces
  - Molecular Dipoles
  - Forces
    - Dipole-Dipole
    - London Forces
    - Hydrogen Bonding



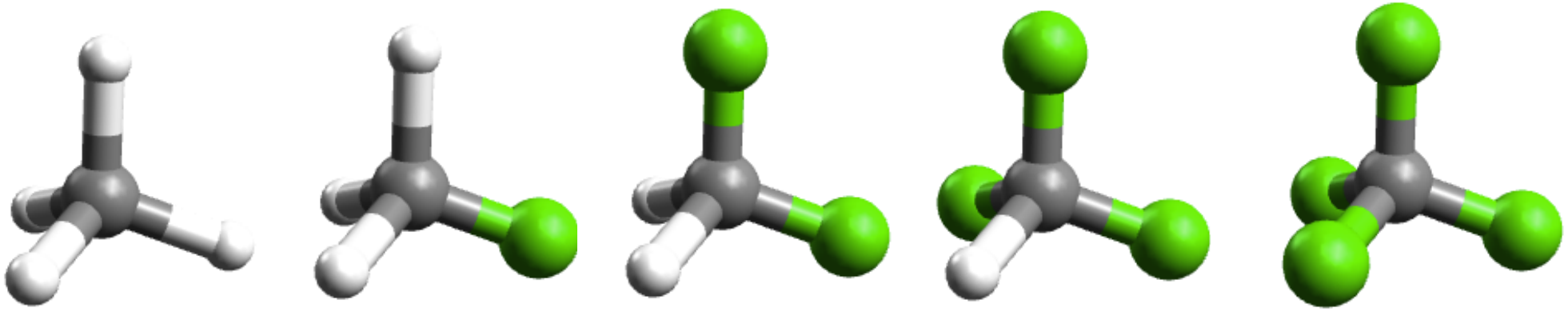




Electronic vs Molecular Geometry

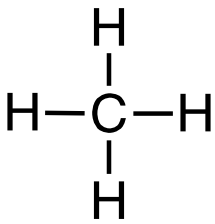


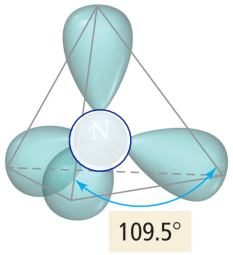
- Electronic geometry is the shape defined by the electron domains.
- Molecular geometry is the shape defined by atoms which *may* be attached to those domains.
- Don't confuse the two!
- There are only five electronic geometries.
- The question "what is the electronic geometry of an atom?" will only have one of these five answers:
  - Linear (two domains)
  - Trigonal Planar (three domains)
  - Tetrahedral (four domains)
  - Trigonal Bipyramidal (five domains)
  - Octahedral (six domains
- If there are 4 electron domains, the electronic structure is tetrahedral.
- With a tetrahedral electronic geometry we could have one atom, two atoms, three atoms, or four atoms stuck onto the central atom.
- A tetrahedral electronic geometry could produce 4 different molecular geometries.

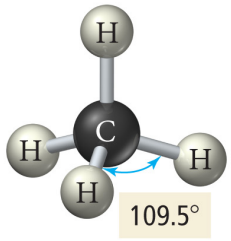


Tetrahedral Electronic Geometry

- There are only five electronic geometries, but each can result in many molecular geometries.
- Only one electronic geometry occurs when there are 4 electron domains.
- But there are multiple molecular geometries that can be built on a tetrahedral electronic geometry.

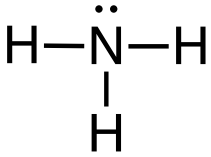


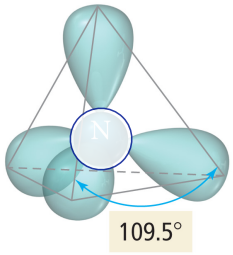


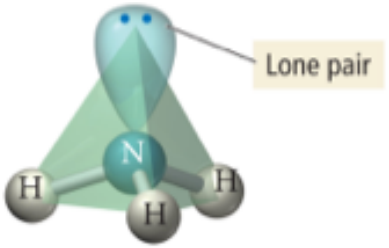


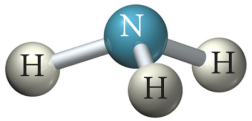
Electronic Geometry: Tetrahedral

Molecular Geometry: Tetrahedral



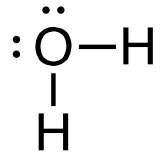


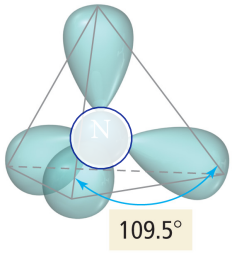


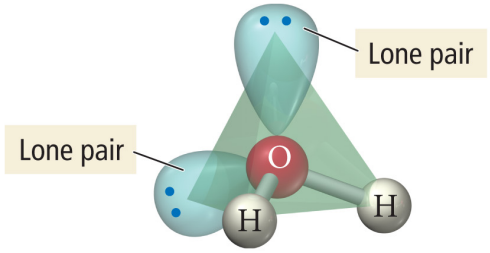


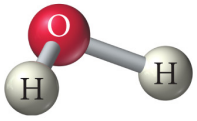
Electronic Geometry: Tetrahedral

Molecular Geometry: Trigonal Pyramidal









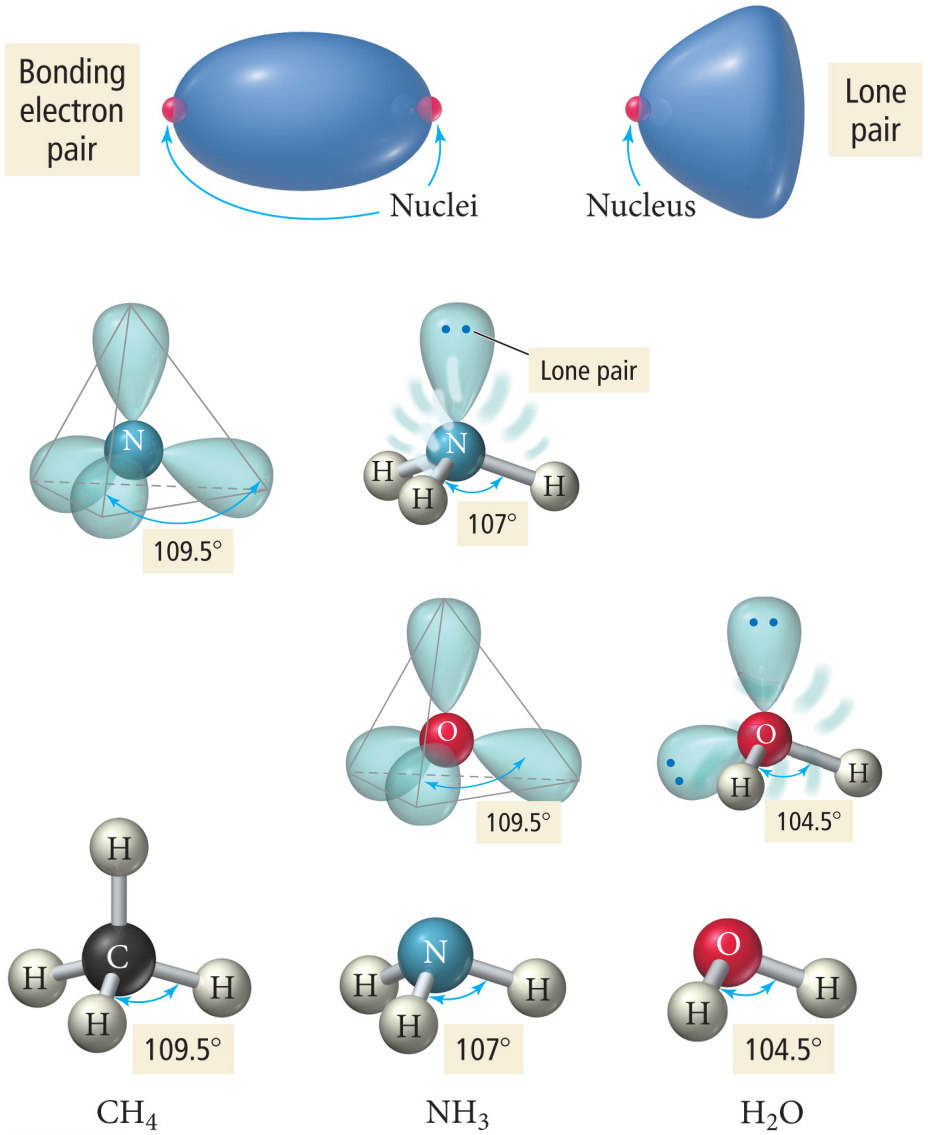
Electronic Geometry: Tetrahedral

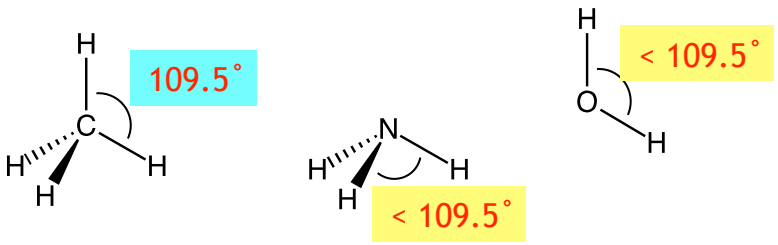
Molecular Geometry: Bent

Bond Angle Compression

- Two electrons, a lone pair, in an electronic domain spread out.
- When those same electrons are in a covalent bond, the nuclei of the two atoms pull them into a smaller area.
- Lone pairs occupy more space than covalent bonds.
- Lone pairs press on adjacent covalent bonds and compress the bond angles between covalent bonds.
- You are responsible for knowing the ideal bond angle of a tetrahedral geometry is 109.5˚
- You are responsible for knowing when bond angle compression produces an angle less than 109.5˚

  Write " < 109.5" when asked to label compressed bond angles.
- You are not responsible for knowing the exact angle of a compressed bond.

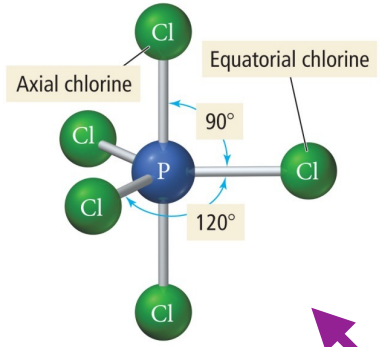




Trigonal Bipyramidal Electronic Geometry

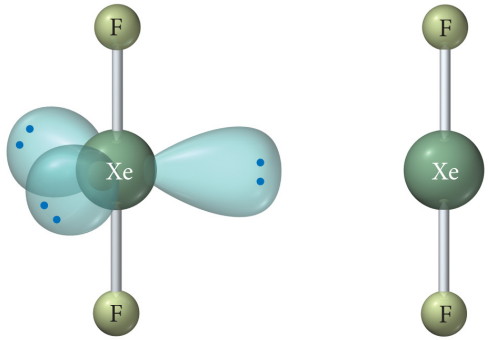
Electronic Geometry:
Trigonal Bipyramidal

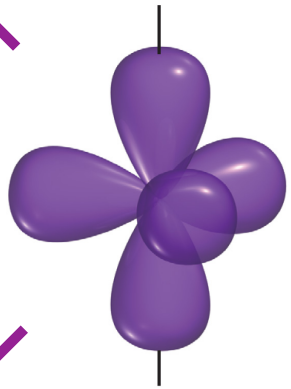
Molecular Geometry:
Trigonal Bipyramidal



Electronic Geometry:
Trigonal Bipyramidal

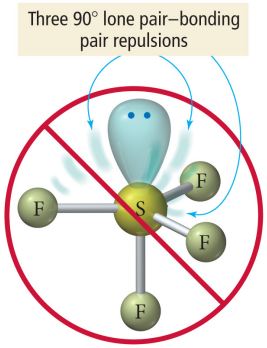
Molecular Geometry:
Linear





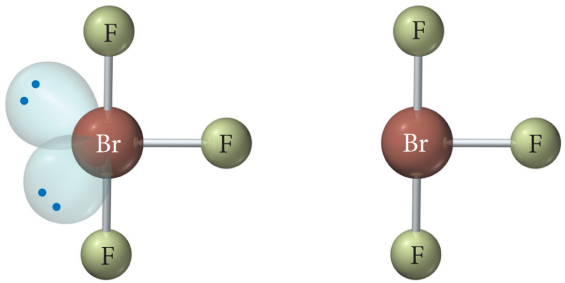
Electronic Geometry:
Trigonal Bipyramidal

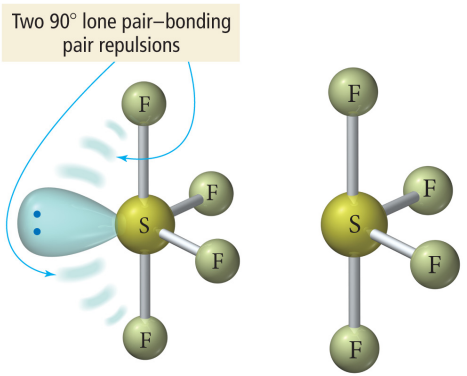
Molecular Geometry:
Seesaw

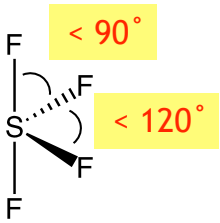


Electronic Geometry:
Trigonal Bipyramidal

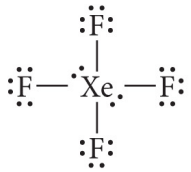
Molecular Geometry:
T-Shaped

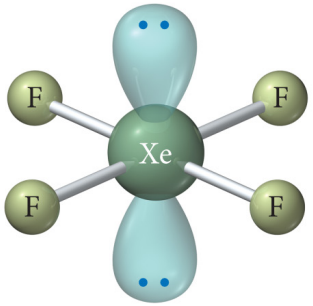


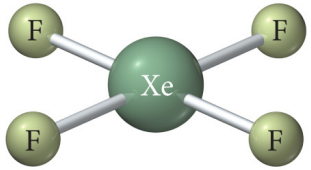




Octahedral Electronic Geometry

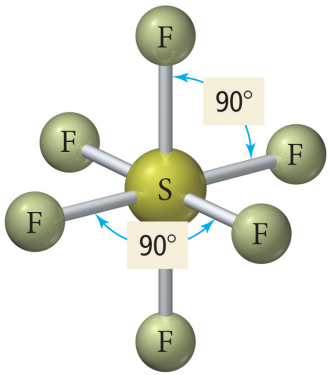


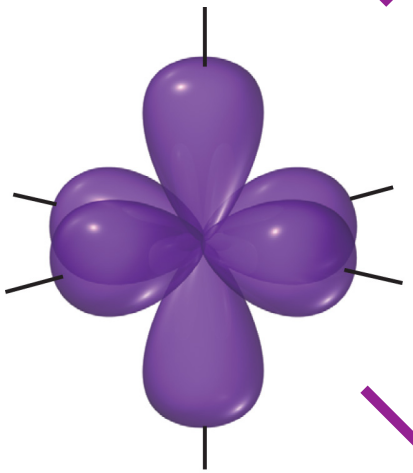


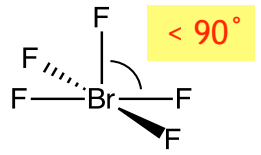


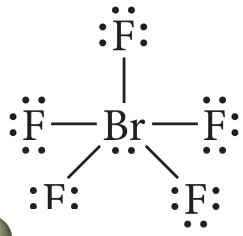
Electronic Geometry:
Octahedral

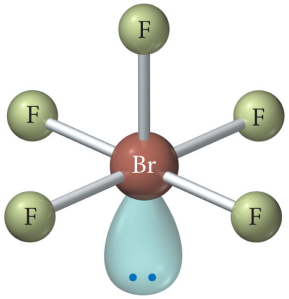
Molecular Geometry:
Square Planar

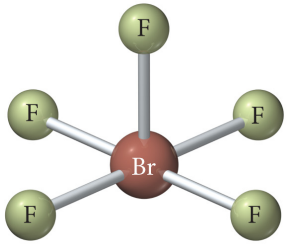












Electronic Geometry:
Octahedral

Molecular Geometry:
Square Pyramidal

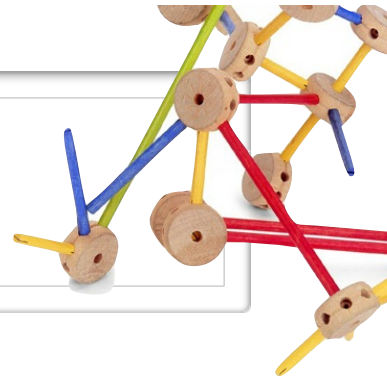
Electronic Geometry:
Octahedral

Molecular Geometry:
Octahedral

	Electronic Geometry	Molecular Geometry	Bond Angles
1 e pair	Linear	Linear	180˚
2 e pair	Linear 	Linear	180˚
		Linear	
3 e pair	Trigonal Planar 	Trigonal Planar	120˚
		Bent	
		Linear	
4 e pair	Tetrahedral 	Tetrahedral	109.5˚
		Trigonal Pyramidal	
		Bent	
		Linear	
5 e pair	Trigonal Bipyramidal 	Trigonal Bipyramidal	90˚ and 120˚
		See-saw	
		T-Shaped	
		Linear	
		Linear	
6 e pair	Octahedral 	Octahedral	90˚
		Square Pyramidal	
		Square Planar	
		T-Shaped	
		Linear	
		Linear	

Ch06

Molecules



- Understanding Molecules
  - The covalent bond.
    - Gilbert Lewis
    - Connectivity
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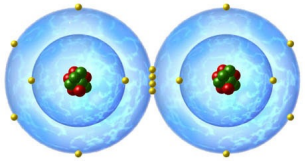
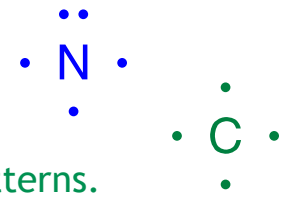
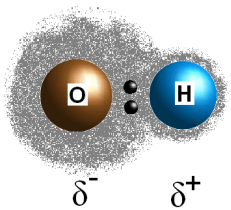
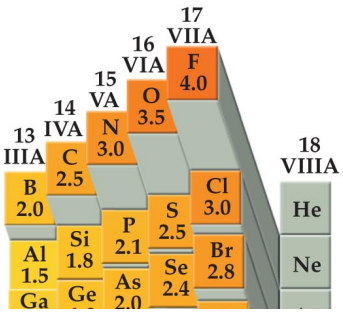
    - Explaining bonding patterns.
- Electronegativity
  - Polar covalent bonds
    - Bond Dipoles
  - Pauling values
    - Reference Values
    - ΔEN Thresholds
      - covalent, ΔEN = 0-0.4
      - polar covalent, ΔEN = 0.4-2.0
      - ionic, ΔEN = 2.0+



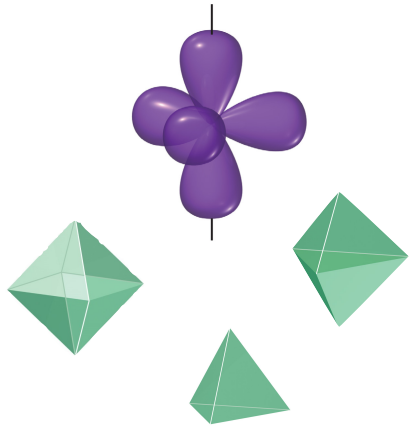


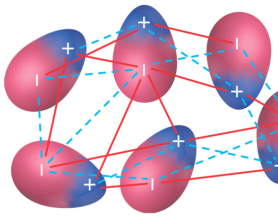


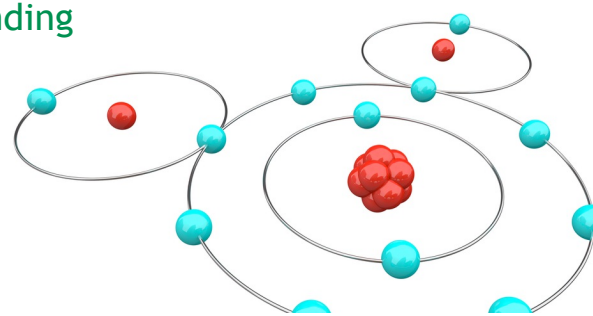


- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
- Molecular Structure
- Intermolecular Forces
  - Molecular Dipoles
  - Forces
    - Dipole-Dipole
    - London Forces
    - Hydrogen Bonding

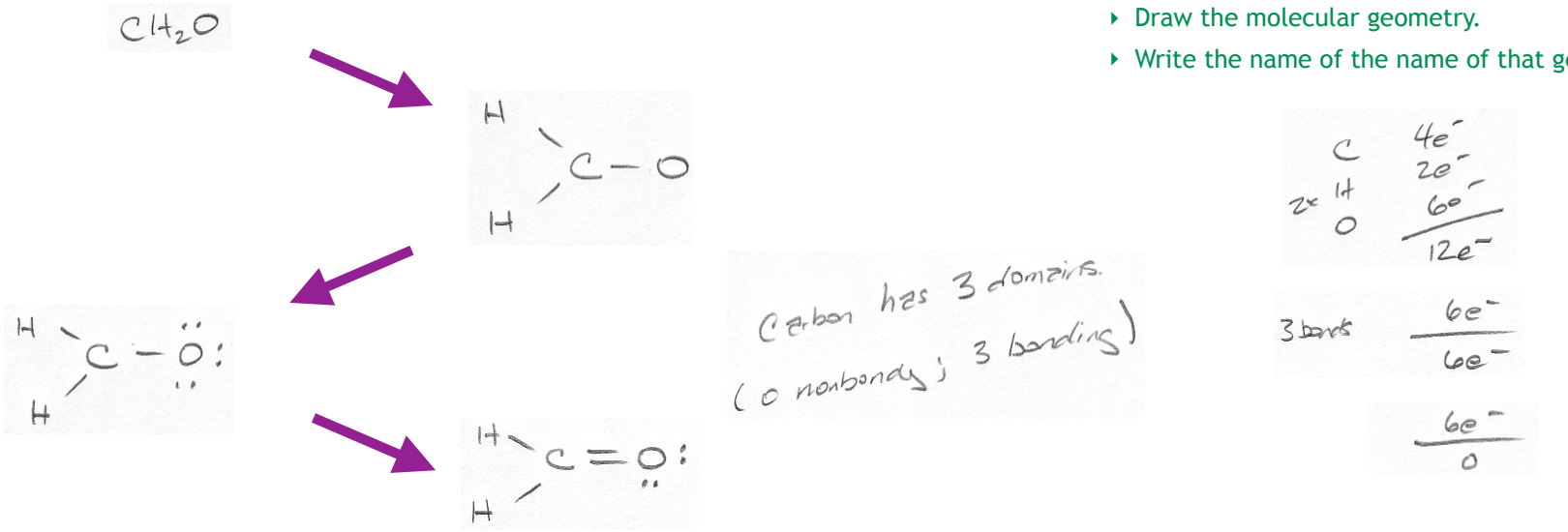


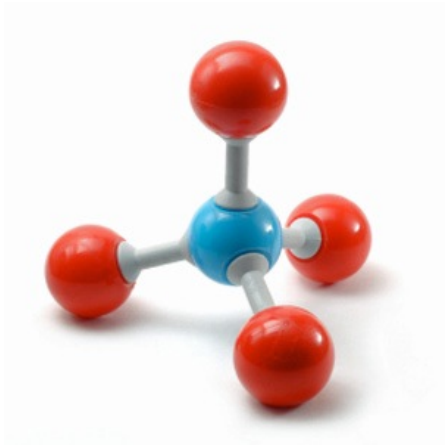




VSEPR Process

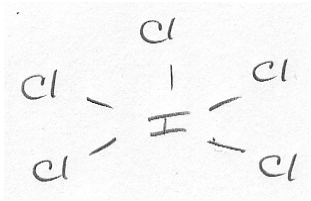
- What is the molecular geometry of carbon in CH_2O?
- To find the molecular geometry of an atom:
  - Draw the Lewis structure.
  - Find the number of domains
    - Which gives you the electronic geometry.
  - Divide the domains into bonding and non-bonding groups.
    - Draw the molecular geometry.
    - Write the name of the name of that geometry.

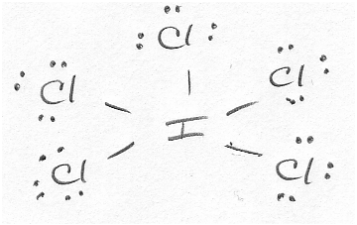


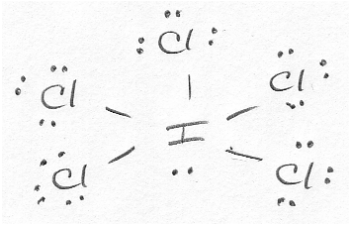


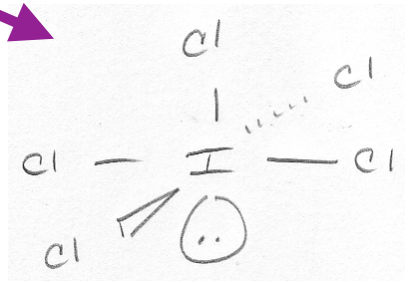
VSEPR Process

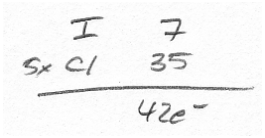
- What is the molecular geometry of iodine in ICl_5?

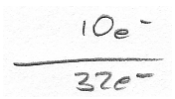


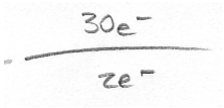












Iodine has 6 domains
(1 non bonding 5 bonding).

Electronic
6 domains → Octahedral

Molecular
5 bonds → Square Pyramidal

- To find the molecular geometry of an atom:
  - Draw the Lewis structure.
  - Find the number of domains
    - Which gives you the electronic geometry.
  - Divide the domains into bonding and non-bonding groups.
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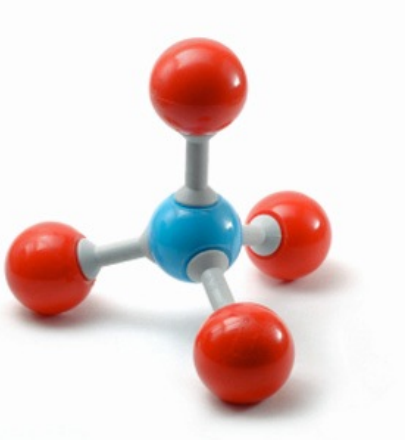
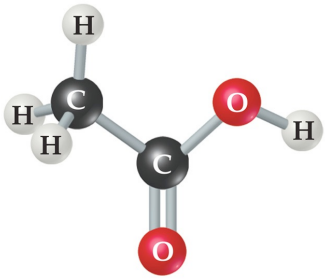
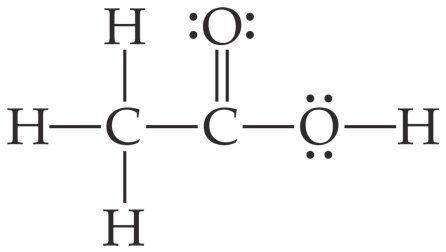
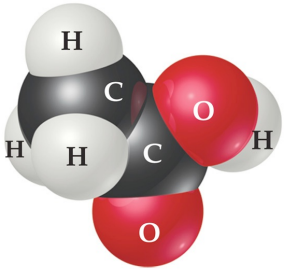


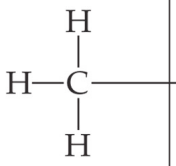
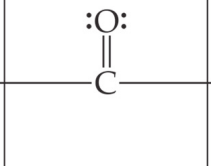
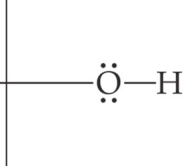
Larger Molecules

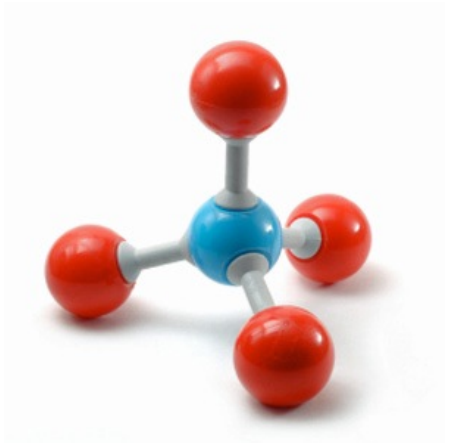
- VSEPR is a tool for understanding the geometry around each atom.
- For larger molecules, sketch out the structure using the Lewis model, and then apply VSEPR separately to each central atom.





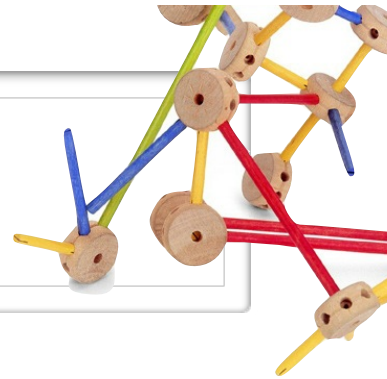


			
Number of electron domains	4	3	4
Electron-domain geometry	Tetrahedral	Trigonal planar	Tetrahedral
Predicted bond angles	109.5°	120°	109.5°



Ch06

Molecules



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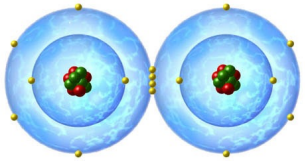

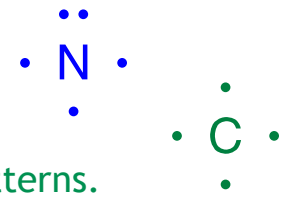

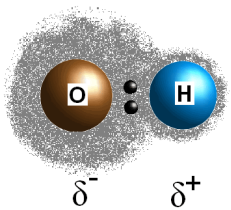

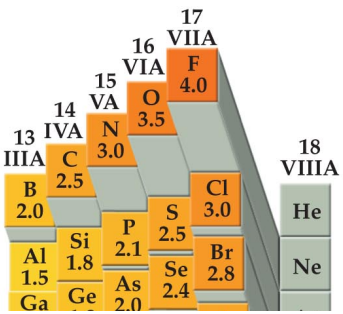

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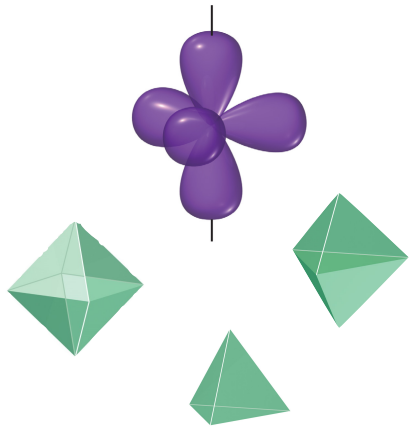
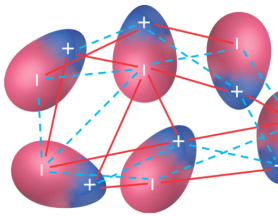
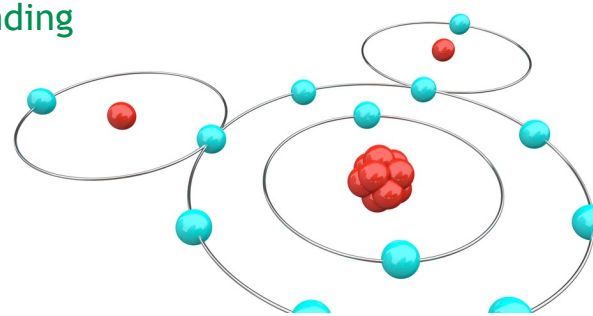
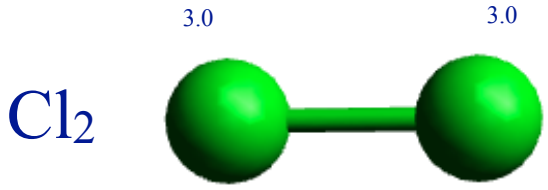




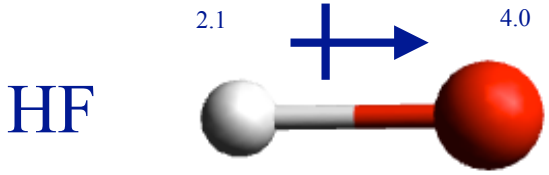


Polar Molecules

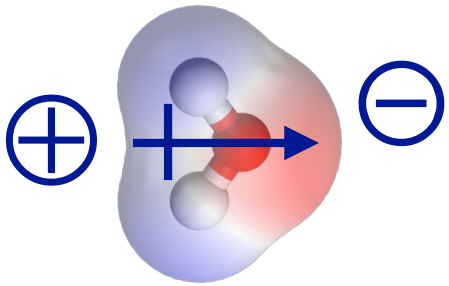
- Bonds can have a dipole moment.
  - A bond dipole is how balanced the electrons in a bond are between two atoms.
  - Bonds that have a dipole moment are said to be polar bonds.
- A molecule can have a net dipole moment.
- The net dipole moment is how balanced the electrons are overall in the entire molecule.
- Molecules that have a net dipole are said to be polar molecules.
- Polar molecules have a “north pole” and “south pole”.
- They interact with electromagnetic fields.
- Including electromagnetic fields of other polar molecules.
- They also have other physical properties unique to polar molecules.
- For example:
  - Polar molecules have higher boiling points.
  - Polar molecules can solvate ions.
  - Polar substances don’t mix with non-polar substances (oil and water).
  - Polar molecules can be affected by magnetic fields (how liquid crystal displays work).

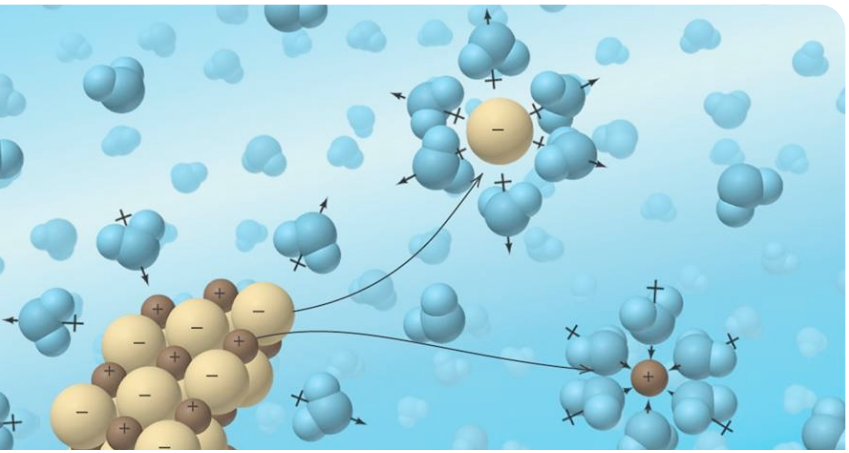


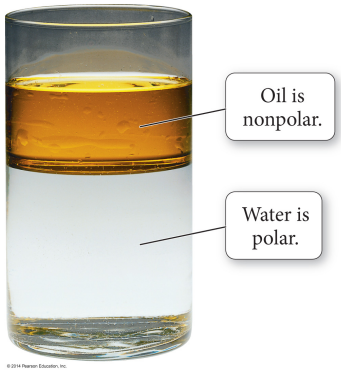
$\Delta EN = 0$

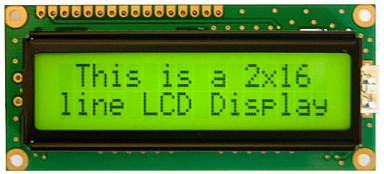


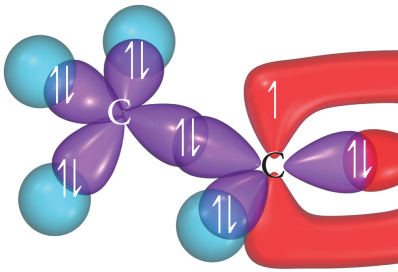
$\Delta EN = 1.9$





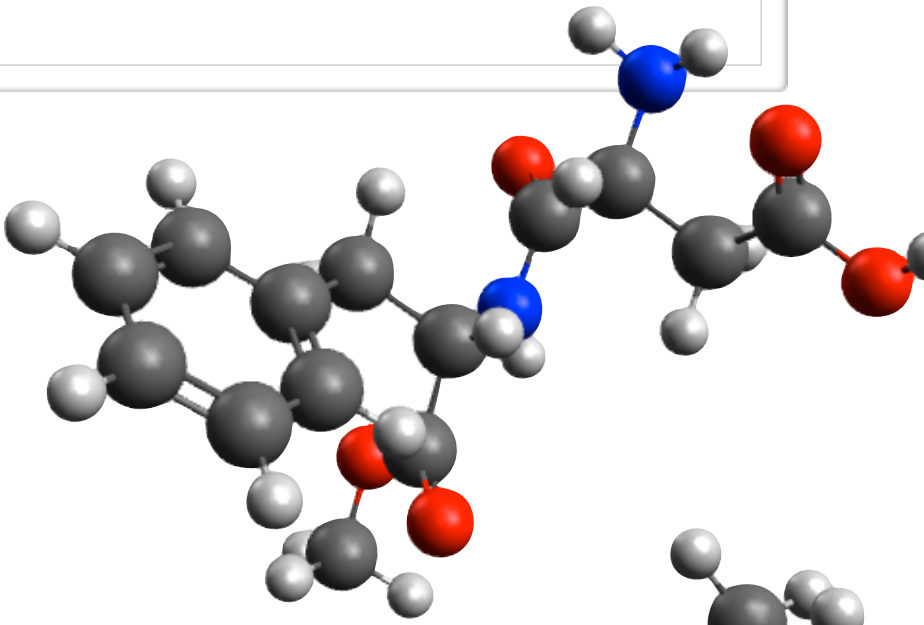


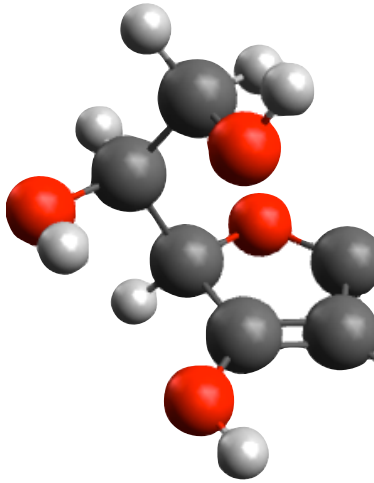


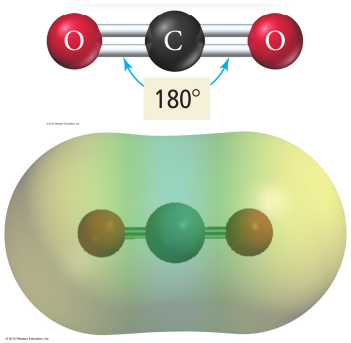


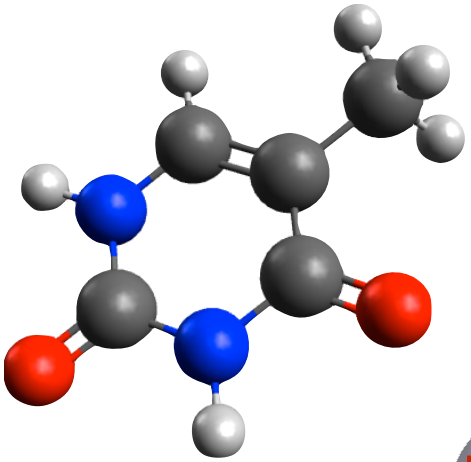
Polar Molecules

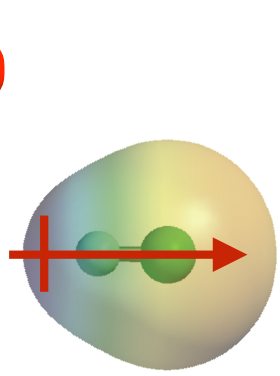
- If there are many bonds, how do you decide if the molecule is polar or non-polar?
- You add up all the bond dipoles in the molecule to create a net dipole.
- Bond dipoles are vectors, we need to talk about vector addition.

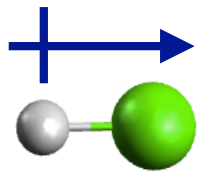


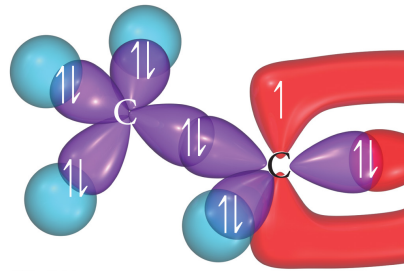






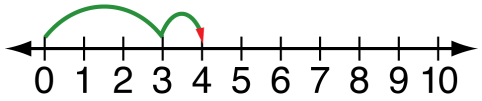


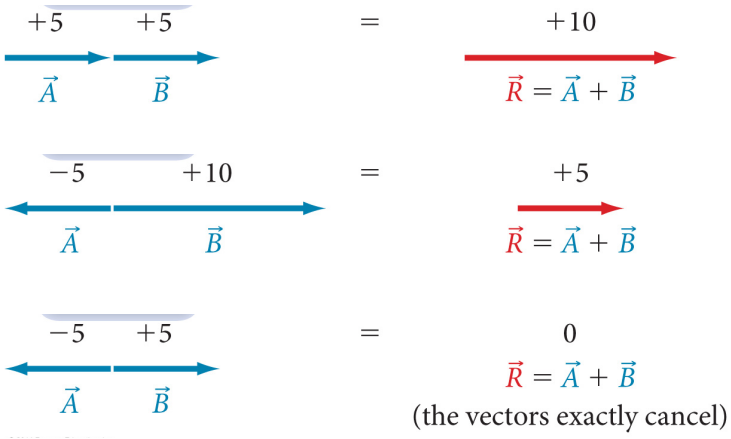




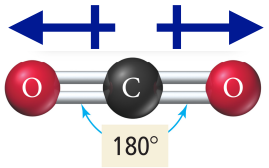
Vector Addition in 1D

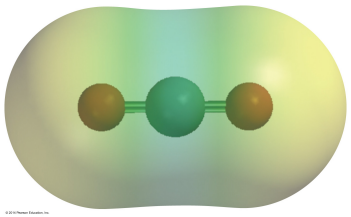
3 + 1 = **4**



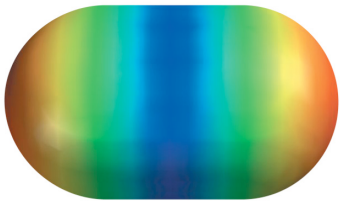


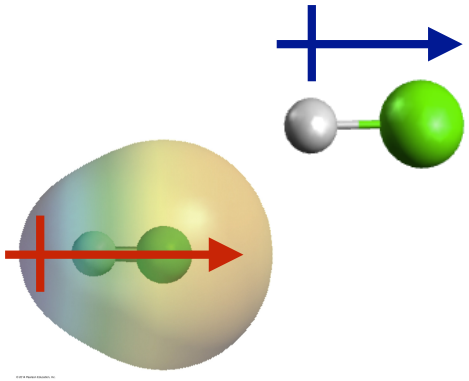
- Dipoles are vectors.
- Vectors have direction and magnitude.
- In grade school, arithmetic is taught using a number line.
- Combining vectors, vector addition, is the same as number line arithmetic.
  - A force of 5 with another force of 5 pointed the same way is a force of 10.
  - A force of 5 with a force of 5 pointed opposite it is 0.
  - A force of 10 with a force of 5 pointed the opposite is a force of 5.
- The individual dipole moments in a molecule contribute to the net dipole moment of the molecule the same way.
  - Dipoles can cooperate or they can cancel.

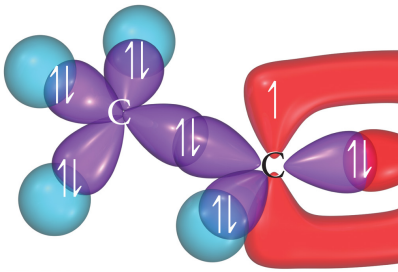




Zero Net Dipole

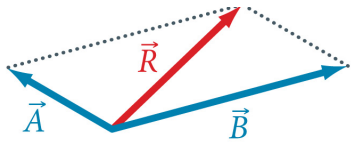




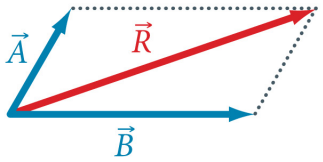


Vectors in 2D Have x and y Components

- When vectors are not on the same number line, it's more challenging to combine them.

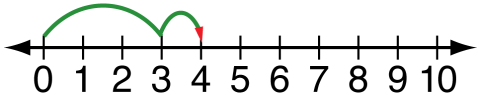


$\vec{R} = \vec{A} + \vec{B}$

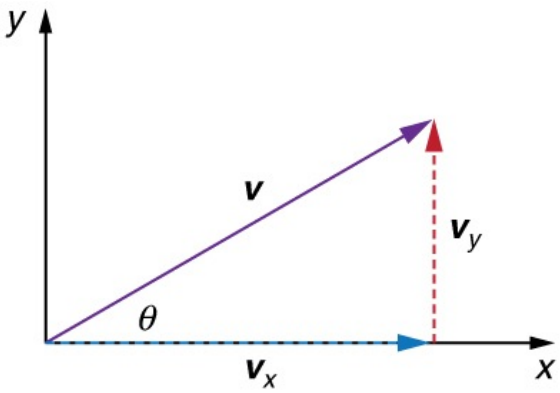


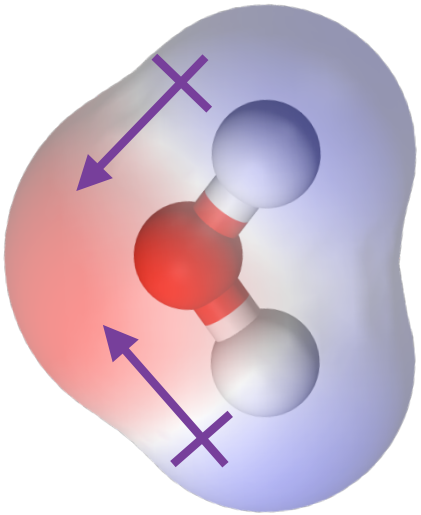
$\vec{R} = \vec{A} + \vec{B}$

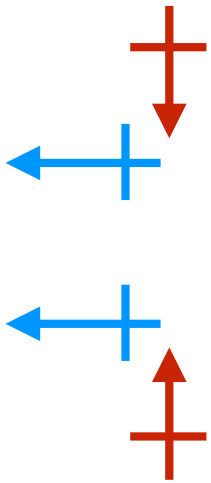
3 + 1 = **4**

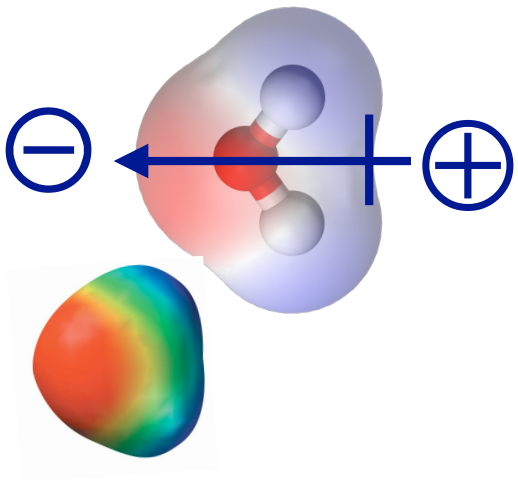


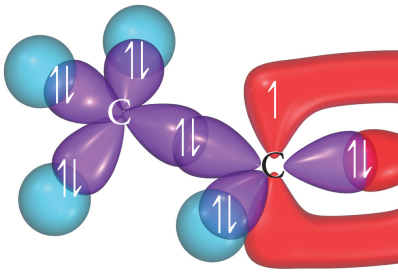
- You need to consider what part of each vector is on the x axis and what part is on the y.
- You can then add each part, just like number line arithmetic.





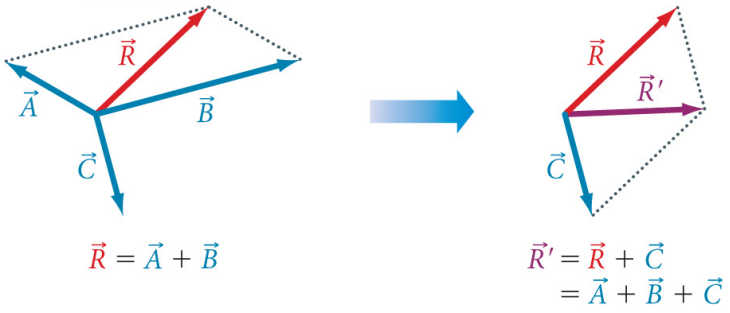


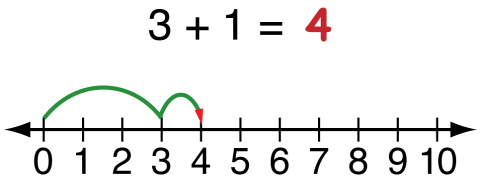


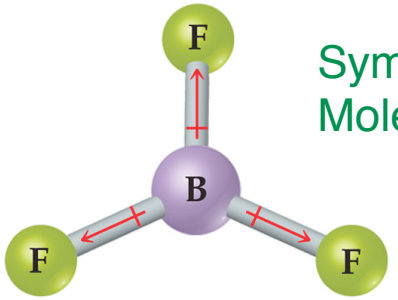


Vectors in 2D Have x and y Components

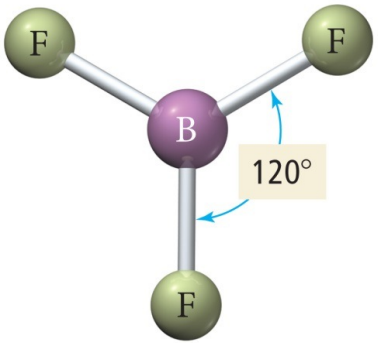
- When vectors are not on the same number line, it's more challenging to combine them.
- If you have 3 or more vectors, sometimes it helps to add two together, then add a third to it, and so on.

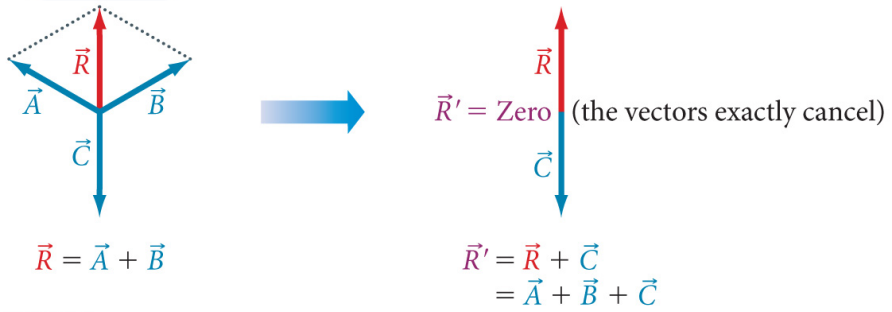


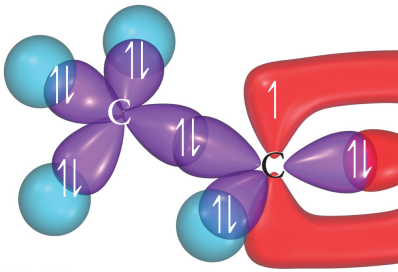




Symmetric Trigonal Planar
Molecules are non-polar

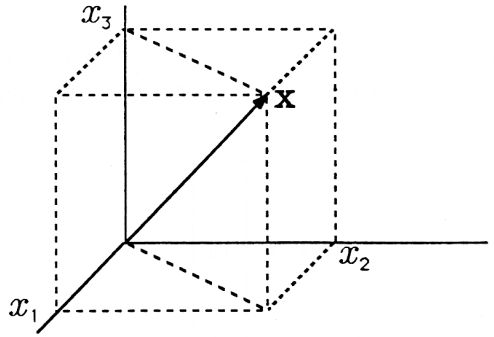


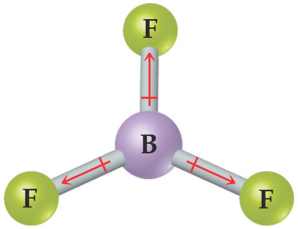




Molecules Exist in 3D Space

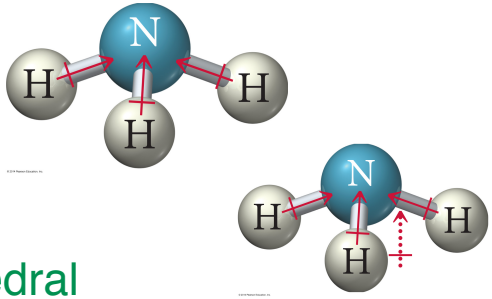
- Molecules are 3D objects.
- We have to consider x, y, and z dimensions of bond dipoles, to understand the net dipole.

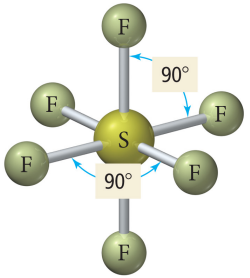


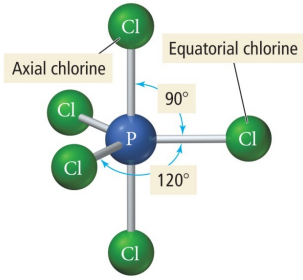


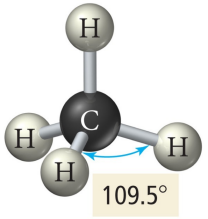
Symmetric Trigonal Planar
Molecules are Non-Polar

Symmetric Trigonal Pyramidal
Molecules are Polar

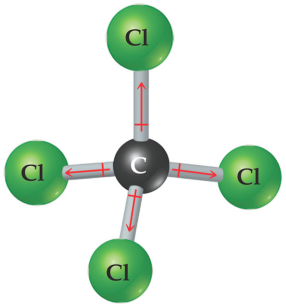


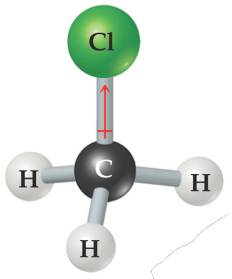




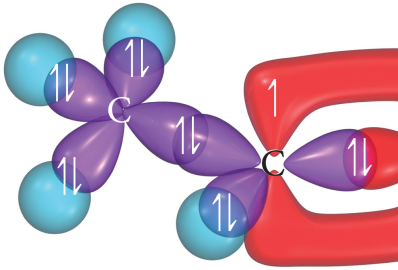


Symmetric Tetrahedral
Molecules are Non-Polar

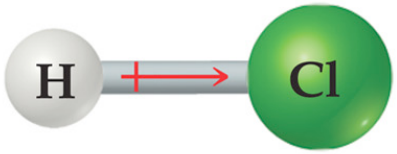




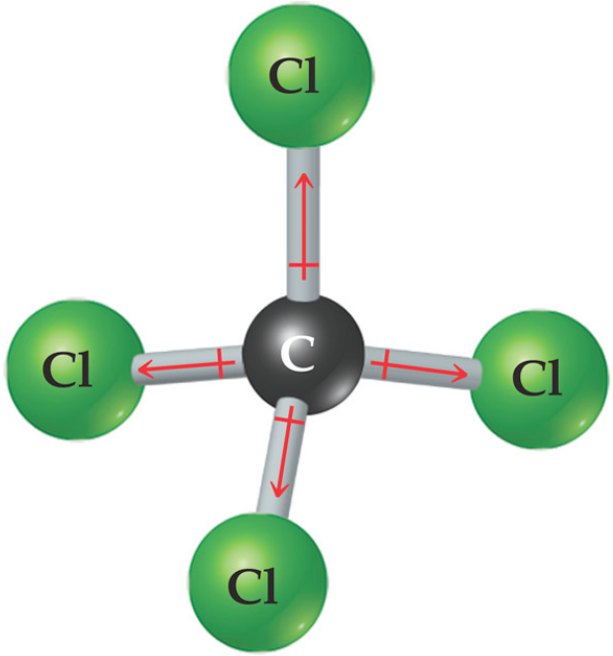
Asymmetric Molecules are
usually Polar.



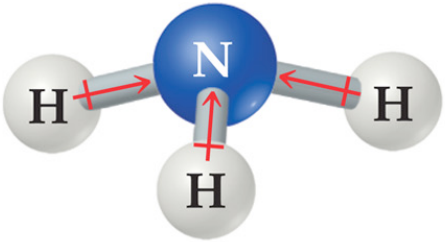
Geometry Affects Polarity



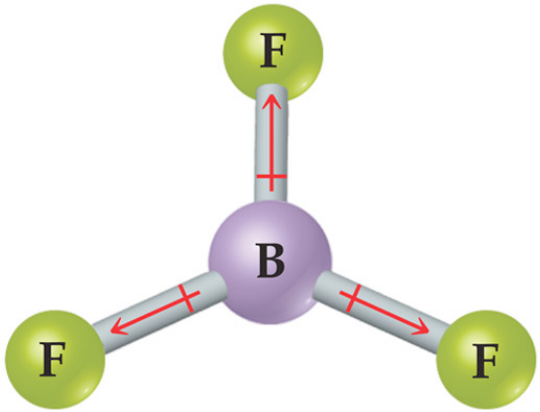
Polar



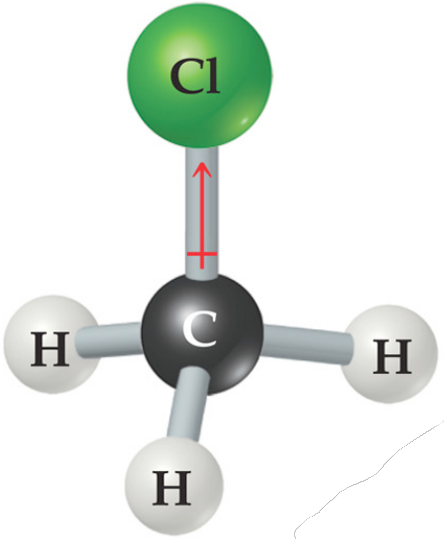
Nonpolar



Polar



Nonpolar



Polar

	Electronic Geometry	Molecular Geometry	Bond Angles
1 e pair	Linear	Linear	180˚
2 e pair	Linear 	Linear	180˚
		Linear	
3 e pair	Trigonal Planar 	Trigonal Planar	120˚
		Bent	
		Linear	
4 e pair	Tetrahedral 	Tetrahedral	109.5˚
		Trigonal Pyramidal	
		Bent	
		Linear	
5 e pair	Trigonal Bipyramidal 	Trigonal Bipyramidal	90˚ and 120˚
		See-saw	
		T-Shaped	
		Linear	
		Linear	
6 e pair	Octahedral 	Octahedral	90˚
		Square Pyramidal	
		Square Planar	
		T-Shaped	
		Linear	
		Linear	

Molecules Exist in 3D Space

- Which molecules or ions are polar?
- Draw the 3D structure, show bond angles, and draw the net dipole for the molecule or ion.

H_2O BrH_5

BCl_3 ClO_2^-

CH_2O PO_4^{3-}

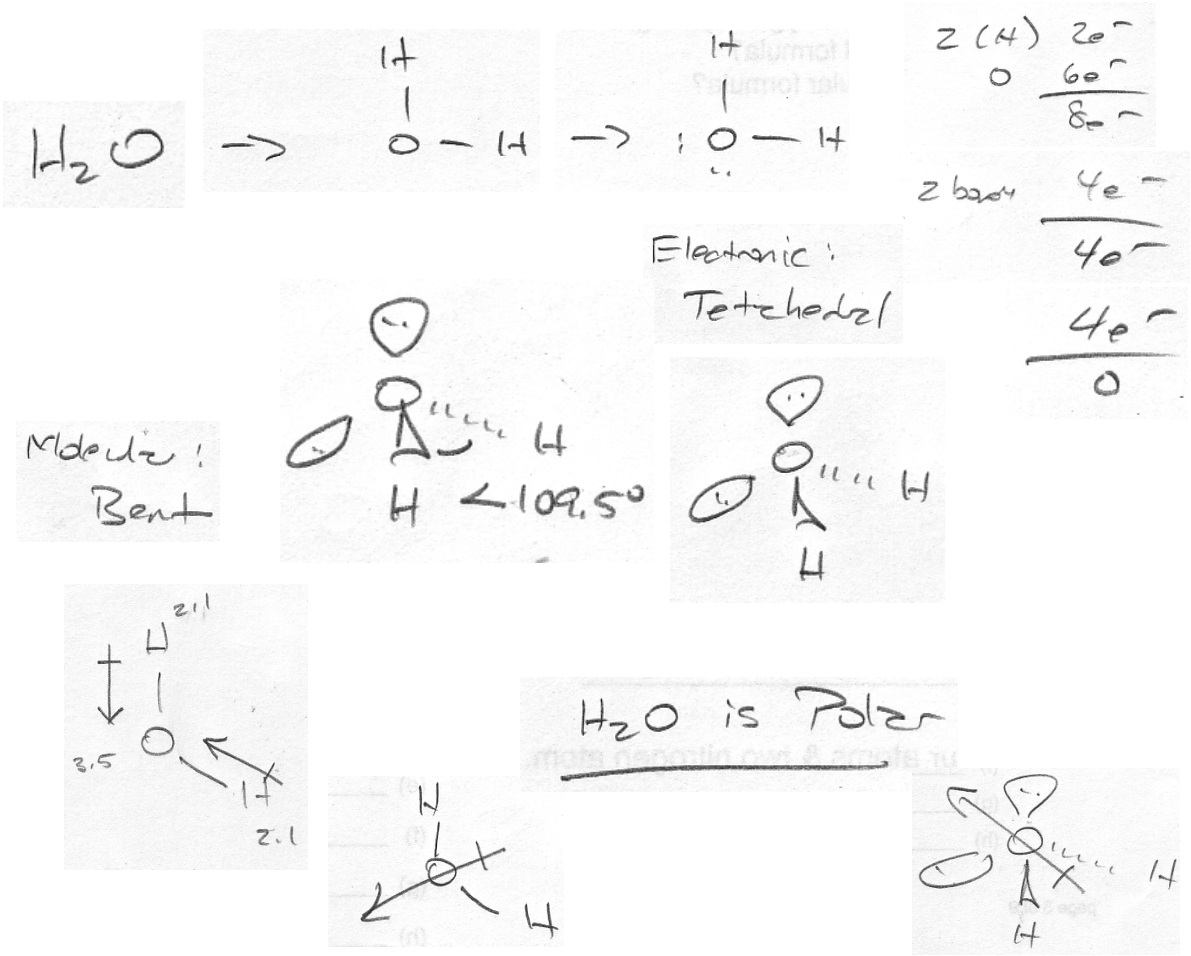
PCl_3 XeF_4

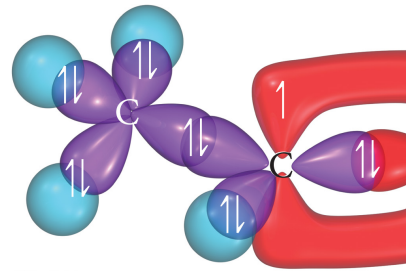
$SClF_5$ SF_4

SO_2

SiO_2

$XeBr_2F_4$





Molecules Exist in 3D Space

- Which molecules or ions are polar?
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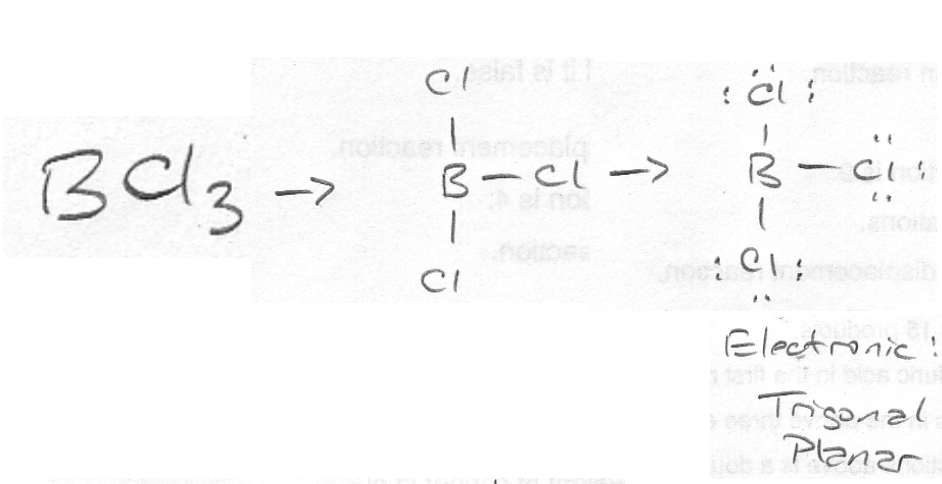

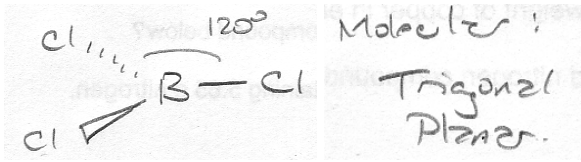

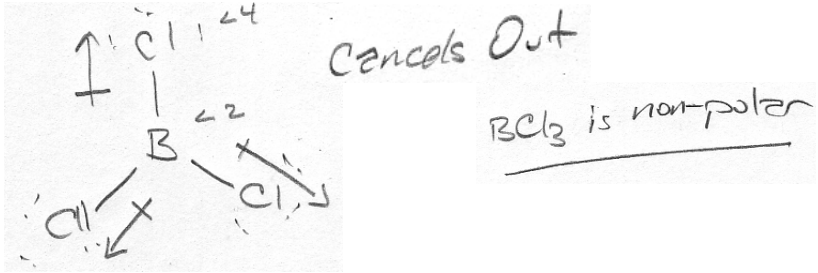

H_2O BrH_5

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CH_2O

PO_4^{3-}

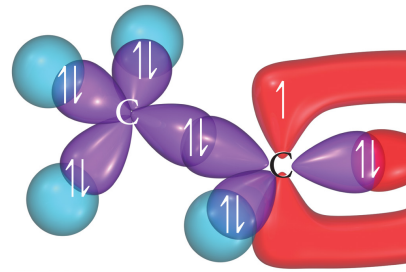
PCl_3 XeF_4

$SClF_5$ SF_4

SO_2

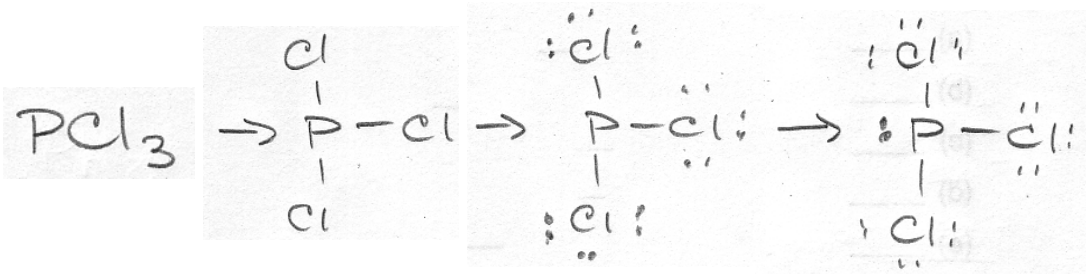
SiO_2

$XeBr_2F_4$



Molecules Exist in 3D Space

- Which molecules or ions are polar?
- Draw the 3D structure, show bond angles, and draw the net dipole for the molecule or ion.



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CH_2O

PO_4^{3-}

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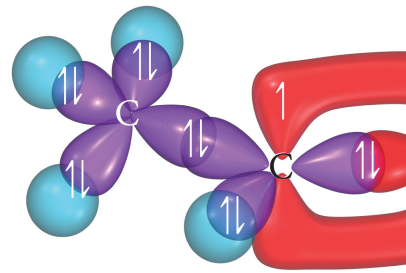
$SClF_5$ SF_4

SO_2

SiO_2

$XeBr_2F_4$



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CH_2O

PO_4^{3-}

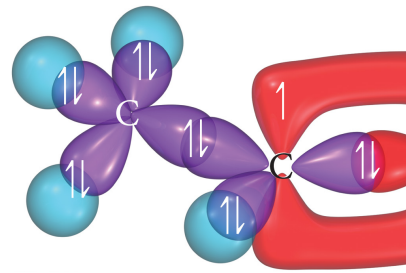
PCl_3 XeF_4

$SClF_5$ SF_4

SO_2

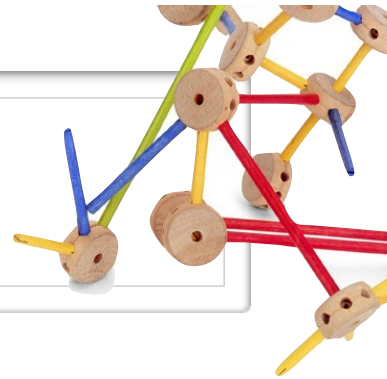
SiO_2

$XeBr_2F_4$



Ch06

Molecules



- Understanding Molecules
  - The covalent bond.
    - Gilbert Lewis
    - Connectivity
  - Lewis Notation
    - Lewis Symbols
    - The octet rule.
    - Explaining bonding patterns.
- Electronegativity
  - Polar covalent bonds
    - Bond Dipoles
  - Pauling values
    - Reference Values
    - ΔEN Thresholds
      - covalent, ΔEN = 0-0.4
      - polar covalent, ΔEN = 0.4-2.0
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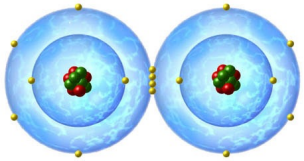
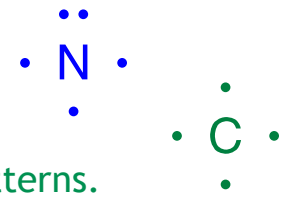
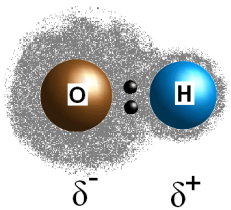
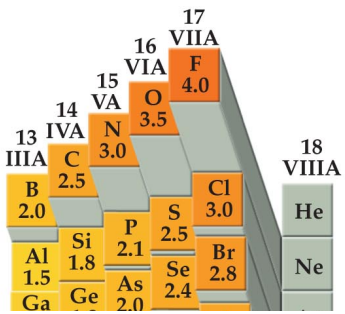


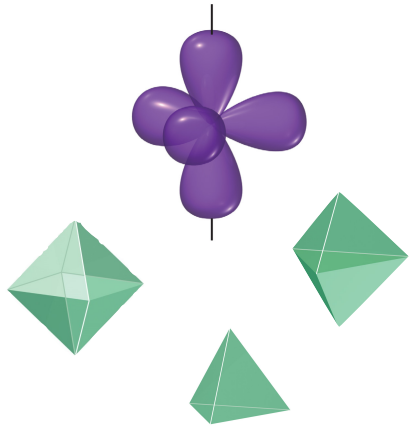




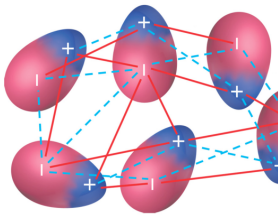


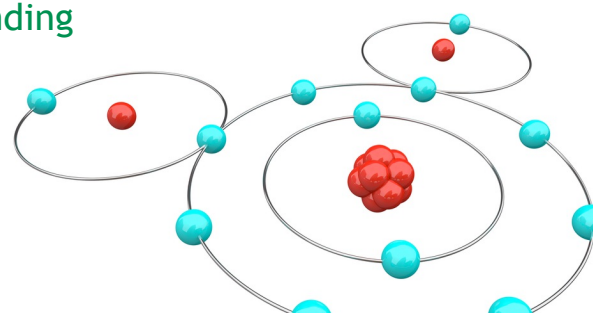
- Lewis Structures
  - Bond order
  - Predicting structures
  - Exceptions

- Molecular Shape
  - Electron Pairs
  - Domains
    - Electronic Structures
  - Molecular Structure



- Intermolecular Forces
  - Molecular Dipoles
  - Forces
    - Dipole-Dipole
    - London Forces
    - Hydrogen Bonding



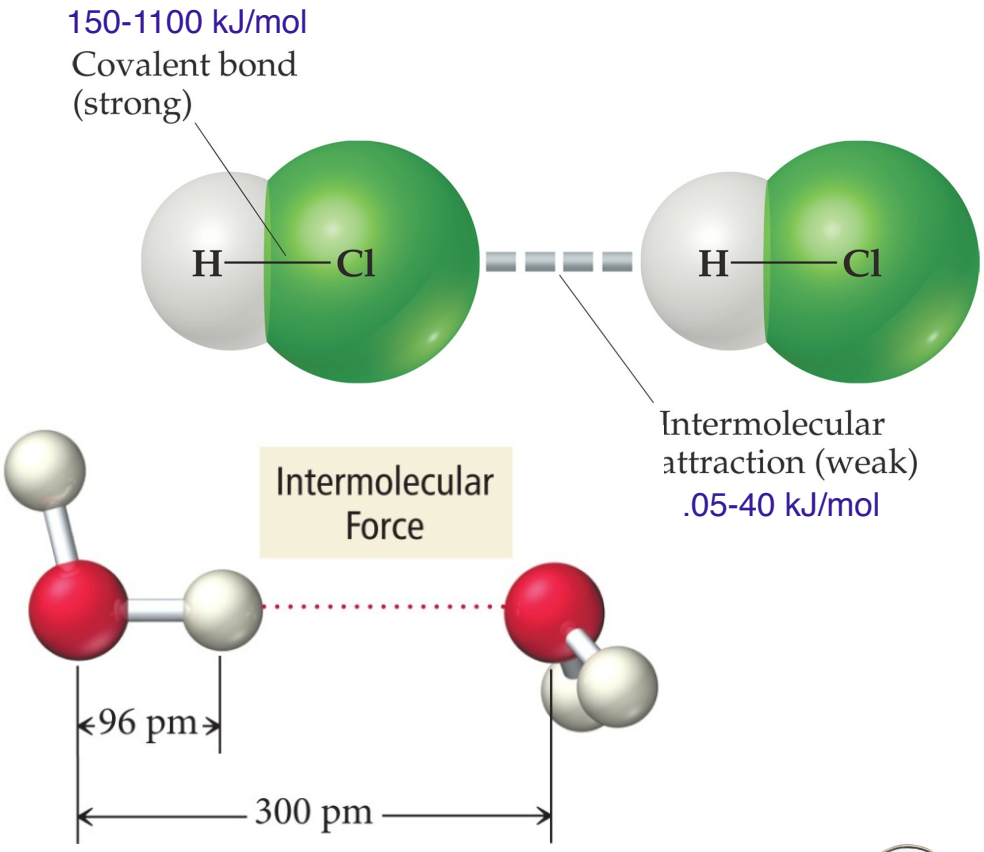


Intermolecular Forces

inTRA — Within a molecule
inTER — Between molecules

- Intermolecular forces are called Van der Walls forces.
- The attractions between molecules are not nearly as strong as the other forces.
- The forces are about 30x less than intermolecular forces.
  - These forces are small, but don't underestimate it's importance.
- Intermolecular forces control many important physical properties:
  - boiling point
  - melting point
  - vapor pressure
  - viscosity
  - hardness
  - surface tension …

greater IF means higher boiling pint, more viscous liquid, harder solid…



"Size matters not … the [intermolecular] force is in everything."

- Yoda, 1980

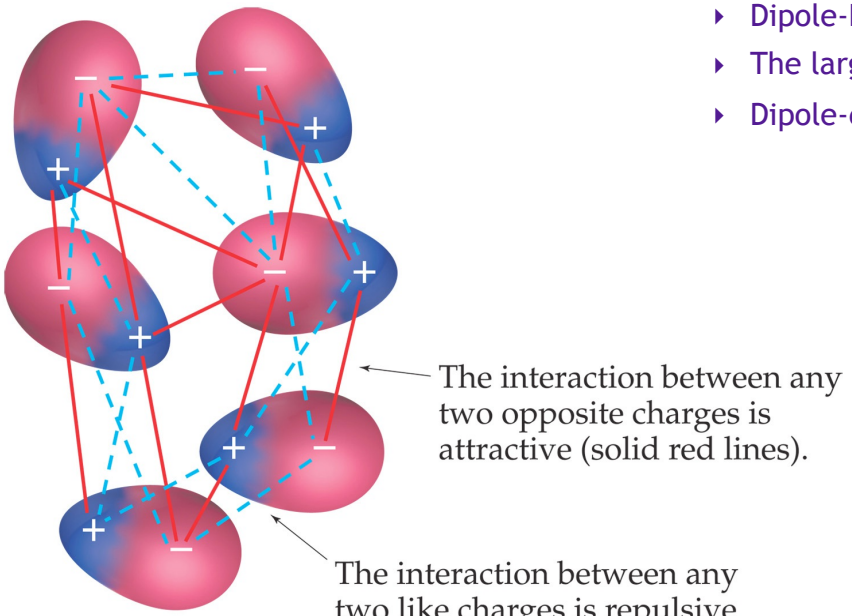
Dipole-Dipole Interactions

There are three intermolecular forces:

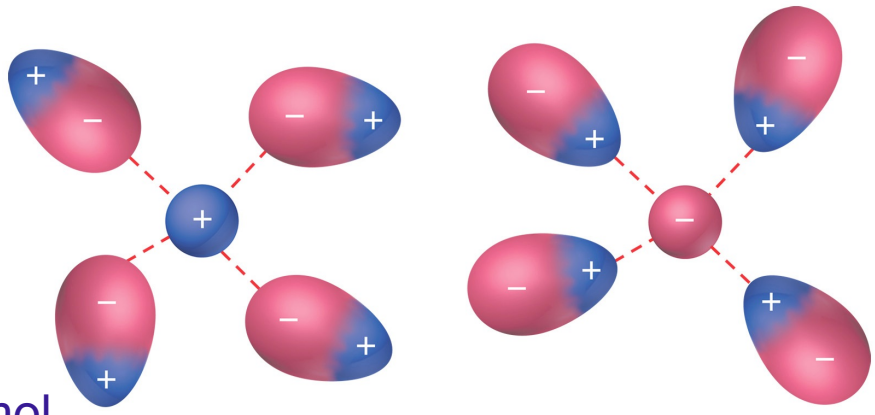
1. Dipole-dipole interactions
2. London-Dispersion forces
3. Hydrogen Bonding

- Ion-dipole interactions (an interparticular force), are important in solutions of ions.
- The strength of these forces are what make it possible for ionic substances to dissolve in polar solvents.
- Molecules that have permanent dipoles are attracted to each other in a similar way.
  - The positive end of one is attracted to the negative end of the other and vice-versa.
  - These forces are only important when the molecules are close to each other.
- Dipole-Dipole forces are weaker than ion-dipole forces.
- The force of attraction is about 5-25 kJ/mol.
- Dipole-Dipole forces increase with a molecules polarity.
- The larger the dipole moment, larger the dipole-dipole force.
- Dipole-dipole interactions exist *only in polar substances*.

5-25 kJ/mol



40-600 kJ/mol



Cation-dipole attractions

Anion-dipole attractions

Dipole-Dipole Interactions

There are three intermolecular forces:

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2. London-Dispersion forces
3. Hydrogen Bonding

Substance	Molecular Weight (amu)	Dipole Moment μ (*D*)	Boiling Point (K)
Propane, $CH_3CH_2CH_3$	44	0.1	231
Dimethyl ether, CH_3OCH_3	46	1.3	248
Methyl chloride, CH_3Cl	50	1.9	249
Acetaldehyde, CH_3CHO	44	2.7	294
Acetonitrile, CH_3CN	41	3.9	355

Dipole-dipole interactions are apparent in trends like boiling point.

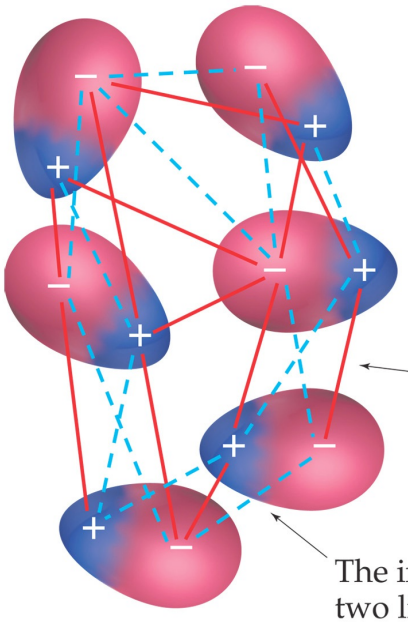
For similar molecules:

the more polar the molecule ⬆

higher intermolecular forces ⬆

the higher is its boiling point ⬆

5-25 kJ/mol



The interaction between any two opposite charges is attractive (solid red lines).

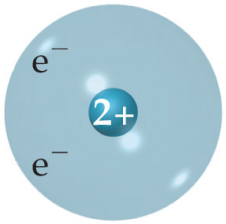
The interaction between any two like charges is repulsive (dashed blue lines).

Dipole-dipole interactions exist only in polar substances!

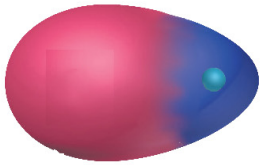
London-Dispersion Forces

There are three intermolecular forces:

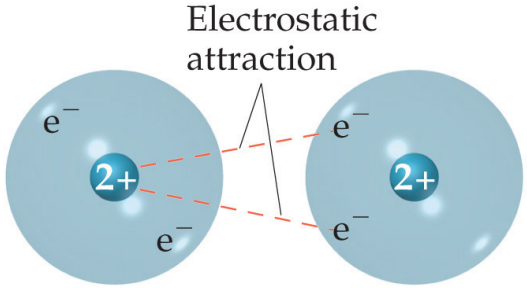
1. Dipole-dipole interactions
2. London-Dispersion forces
3. Hydrogen Bonding



Helium atom

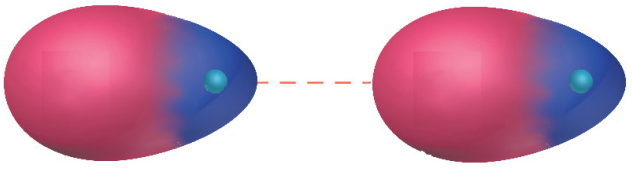


- While the electrons in the 1s orbital of helium would repel each other (and, therefore, tend to stay far away from each other), it does happen that they occasionally wind up on the same side of the atom.
- At that instant, then, the helium atom is polar, with an excess of electrons on the left side and a shortage on the right side.
- If it's close enough, adjacent helium atoms could be effected by that momentary dipole.
- The electrons on the left side of helium atom 2 repel the electrons in the cloud on helium atom 1.
- Even though the two atoms are not polar overall, the momentary shift in electrons causes them both become polar for a very short time — and that polar moment causes them to be attracted.
- London dispersion forces (or just dispersion forces), are attractions between an instantaneous dipole and an induced dipole.
- These forces are present in all molecules, whether they are polar or nonpolar.
- The tendency of an electron cloud to distort in this way is called polarizability.



Helium atom 1 Helium atom 2

.05-40 kJ/mol



London-Dispersion Forces

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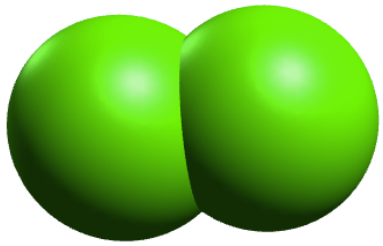
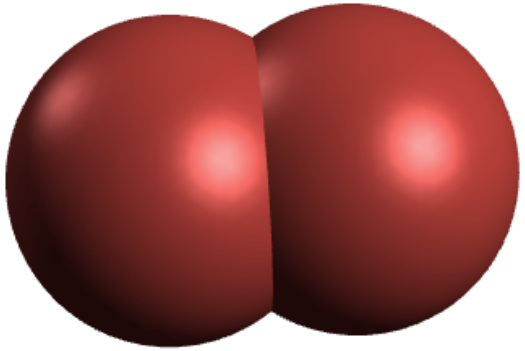
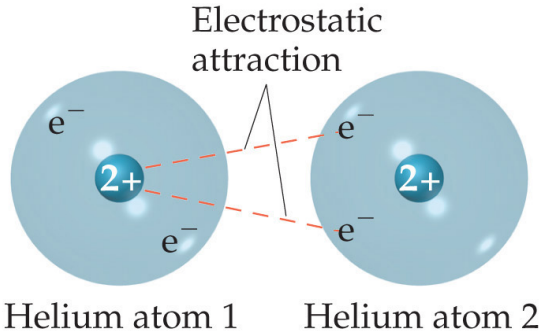
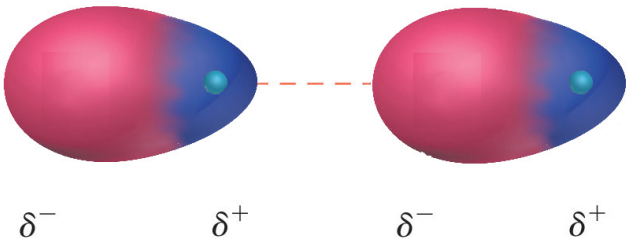






- Dipoles are relative to both the charge and the distance between them.
- Molecules with a large surface area can have greater distance between the momentary charges on their surface.
- So molecules with a greater surface area have greater dispersion forces.
- Br_2 has greater dispersion forces than Cl_2
- Br_2 therefore has a higher boiling point.
- Mass is usually relative to surface area, so you can usually say molecules with more mass will have higher dispersion forces.
- Therefore molecules with higher mass will be more viscous, higher boiling, etc.

Halogen	Molecular Weight (amu)	Boiling Point (K)	Noble Gas	Molecular Weight (amu)	Boiling Point (K)
F_2	38.0	85.1	He	4.0	4.6
Cl_2	71.0	238.6	Ne	20.2	27.3
Br_2	159.8	332.0	Ar	39.9	87.5
I_2	253.8	457.6	Kr	83.8	120.9
			Xe	131.3	166.1



London-Dispersion Forces

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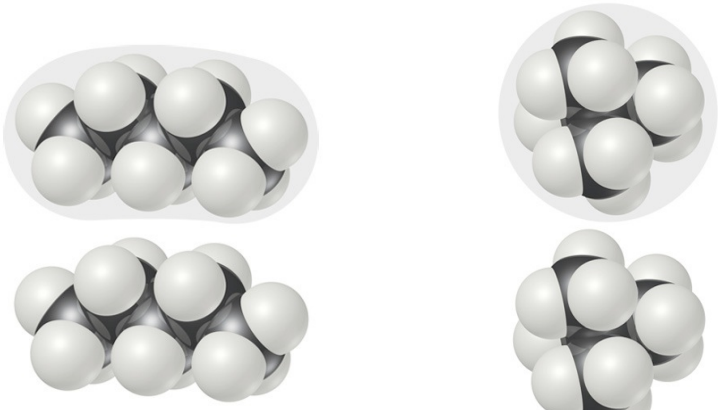
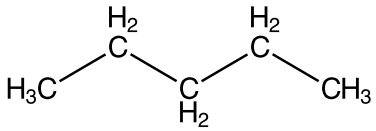
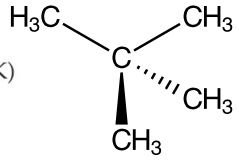
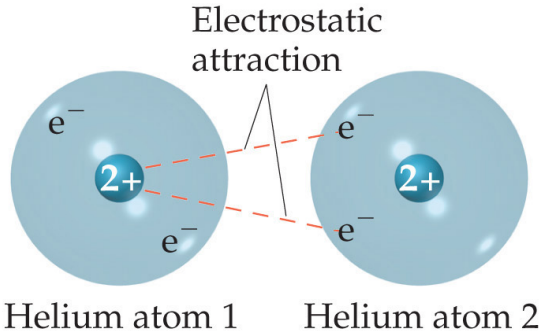


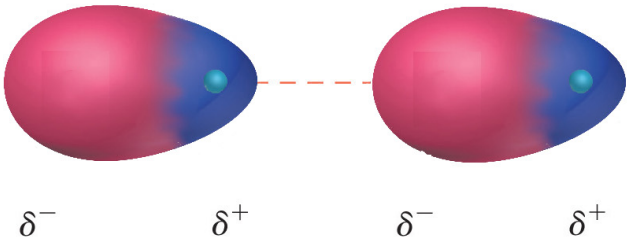




- Shape is also important.
- Two molecules with the same mass may have different surface areas depending on their shape.
- For example molecules with more branches produce more compact shapes.
- They have less surface area, therefore less dispersion forces.
- And lower boiling points.

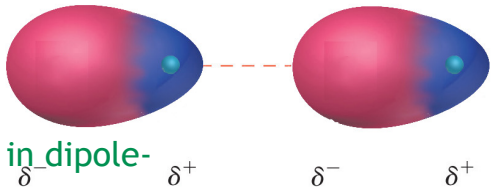


.05-40 kJ/mol

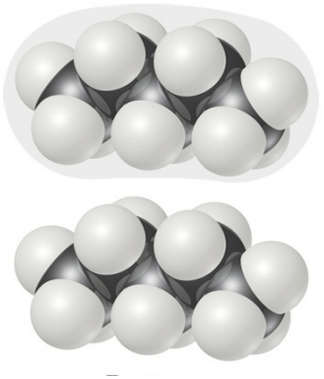


Finding which molecule has greater IF

- All molecules have dispersion forces, but only some have dipole-dipole forces. A polar molecule will usually have greater IF than a non polar one.
- If both molecules are polar:
  - Differences in EN effect IF.
    - Polarity can be influenced by differences in electronegativity.
    - Small changes in ΔEN have big impact on dipoles, therefore big impact in dipole-dipole forces.



  - Symmetry can effect IF.
    - Polarity can be influenced by shape.
    - Symmetric molecules with have less polarity than asymmetric ones.



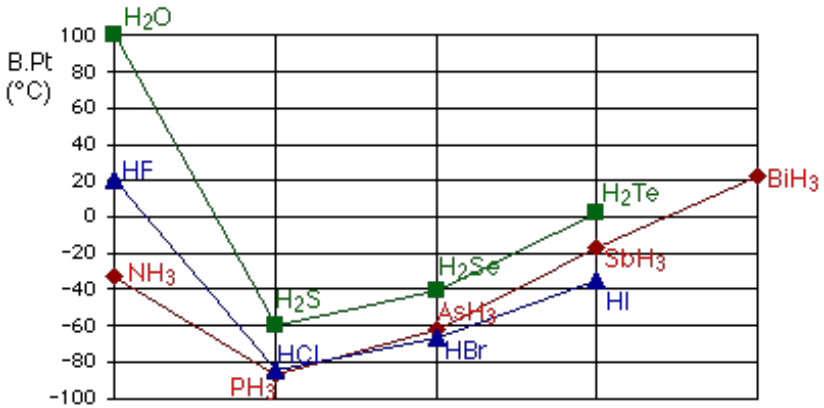
- If both molecules are non-polar:
  - Mass can be an indicator of IF.
    - Greater mass generally corresponds to greater surface area, therefore greater dispersion forces.
  - Branched molecules have lower IF.
    - More branched molecules tend to be more compact, therefore lesser surface area and lesser dispersion forces.

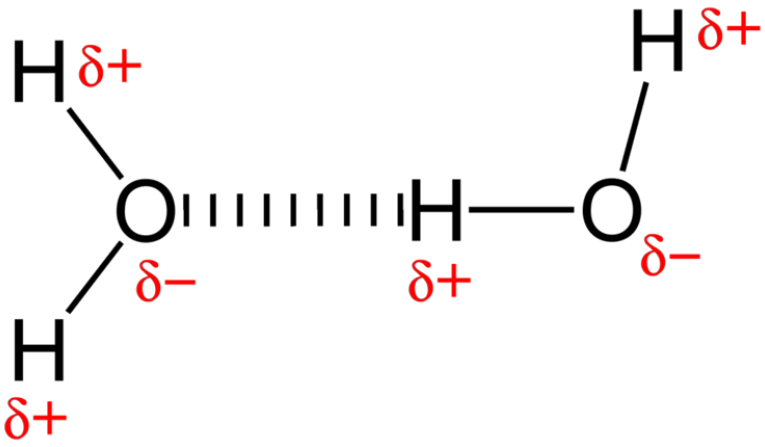
- Differences in IF can indicated differences in boiling point, viscosity, hardness, and more…

Hydrogen Bonding

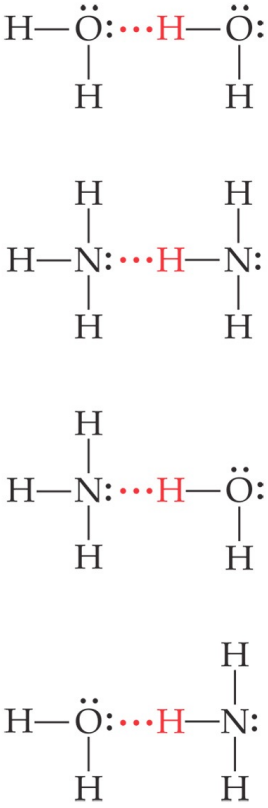
There are three intermolecular forces:

1. Dipole-dipole interactions
2. London-Dispersion forces
3. Hydrogen Bonding





- Whenever a molecule has a bond between H and F, O, or N we see very strong IF forces.
- F, O, and N are the most electronegative elements.
- They pull so much electron density away from the hydrogen that it leaves it almost a bare proton.
- Then we get electrostatic at action between the exposed hydrogen and F, O, and N in adjacent molecules.



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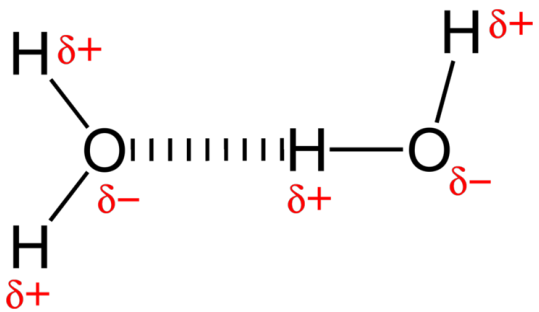
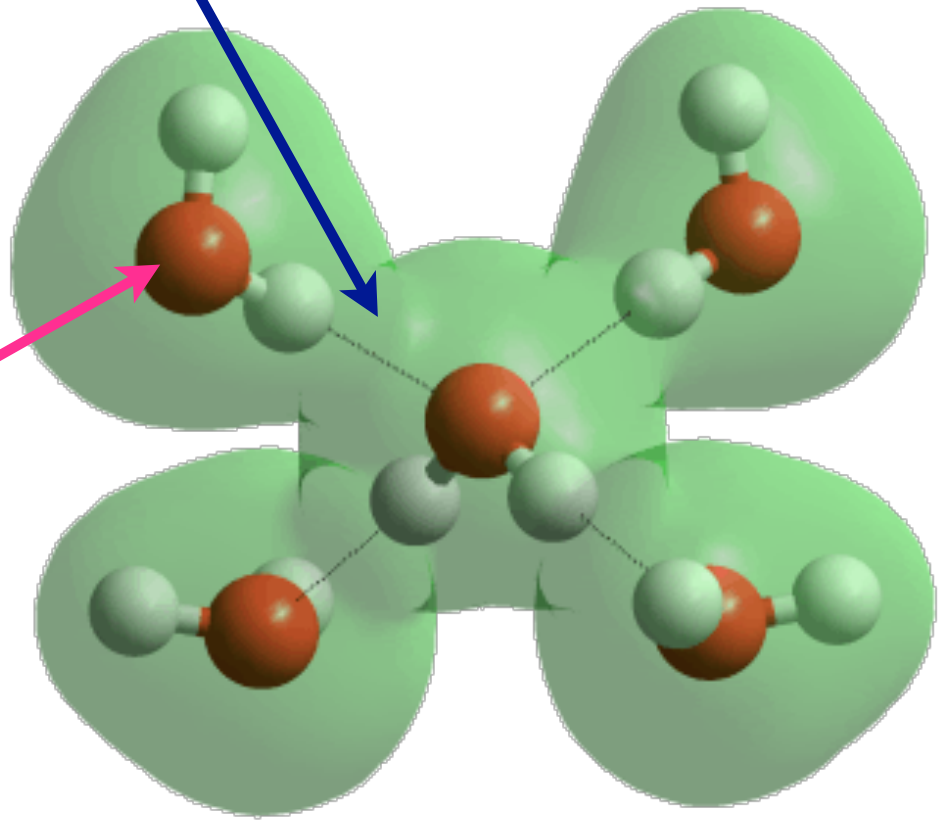


O,N & F are very electronegative so they have strong negative charge for the other molecules hydrogen to be attracted to.

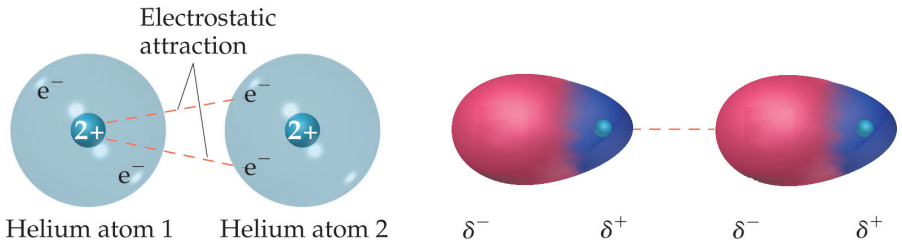
10-40 kJ/mol

That same high electronegatively causes them to strip their own hydrogens of electrons, exposing the positively charged nucleous. Making their hydrogens more hungry for negative charge.



Hydrogen Bonding

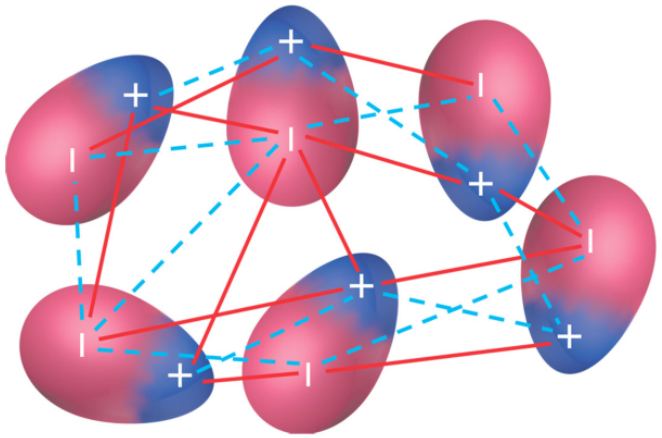
- If hydrogen bonding exists in a molecule, it will be the most important factor in considering IF.



Dispersion

in all molecules

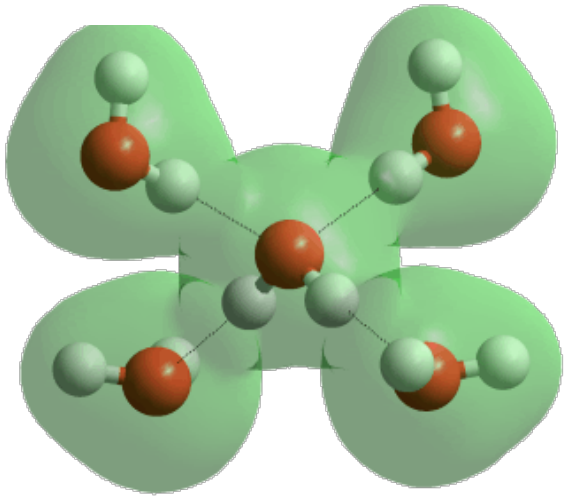
05-40 kJ/mol



Dipole-Dipole

only in Polar Molecules

5-25 kJ/mol



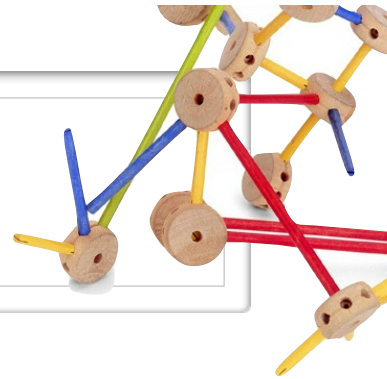
Hydrogen Bonding

only in molecules with OH, NH, or FH

10-40 kJ/mol

Ch06

Molecules



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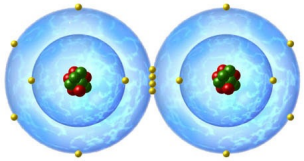

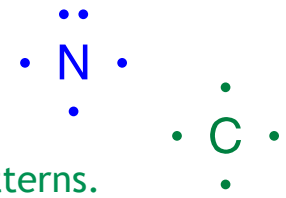

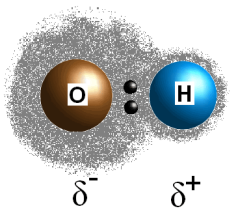

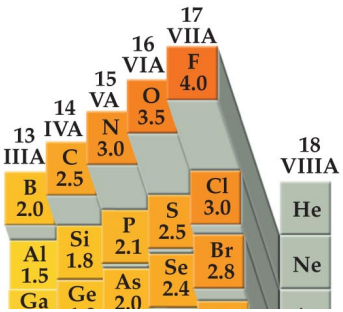

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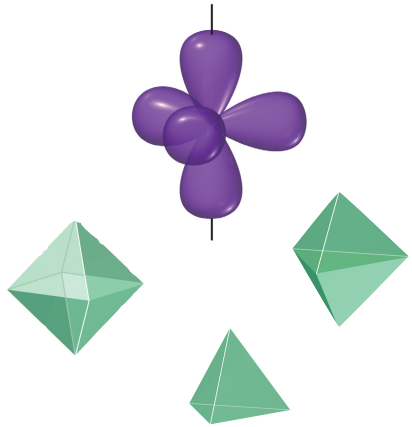

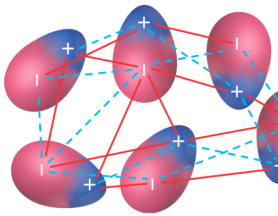

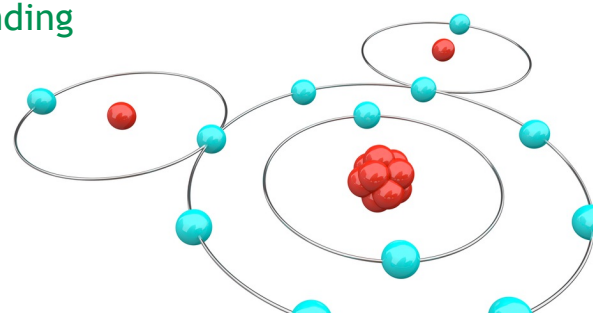

Questions?