Ch12

Chemical Bonds

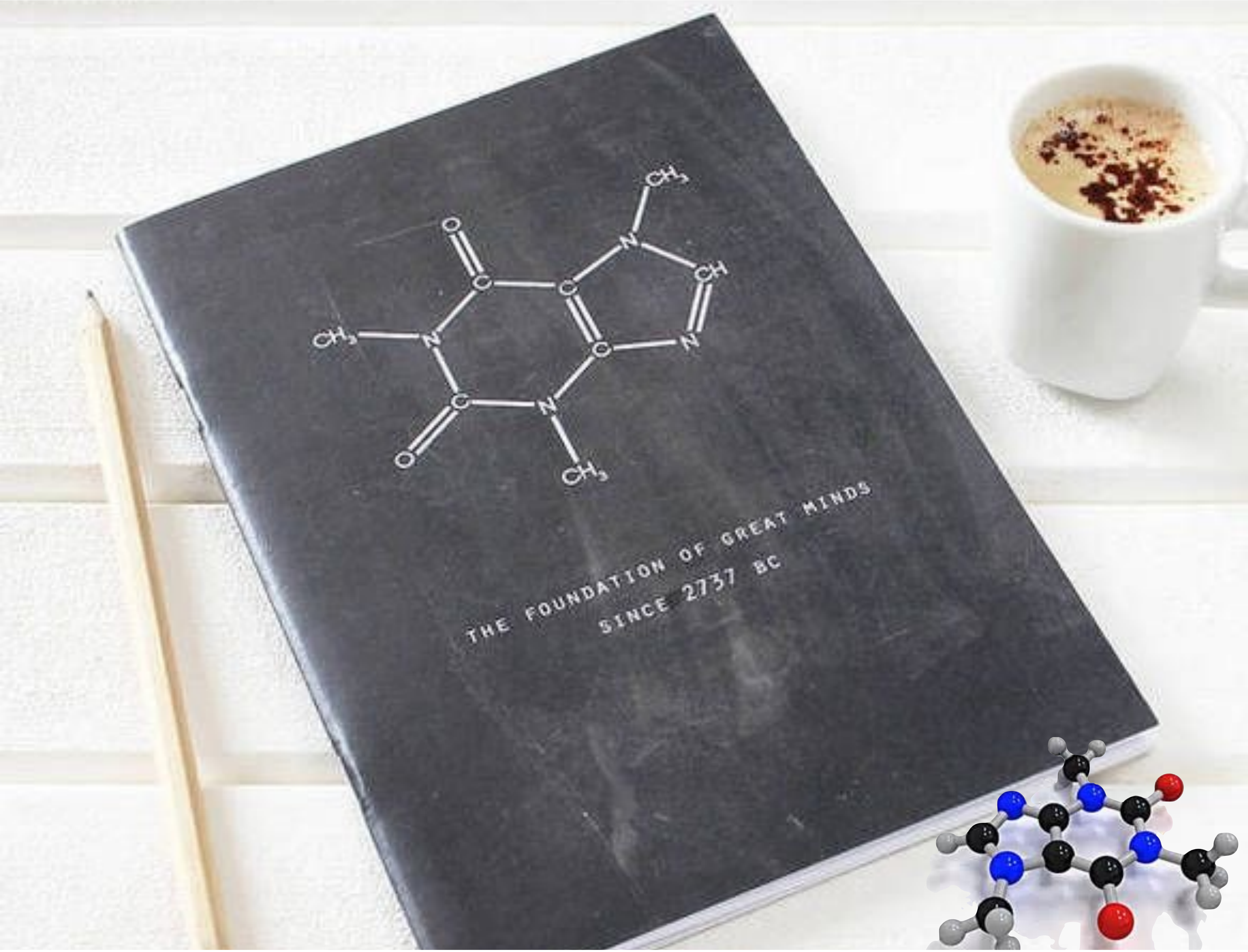
How atoms connect to form … everything.

“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

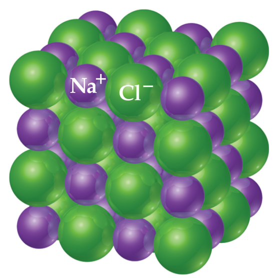
version 1.5

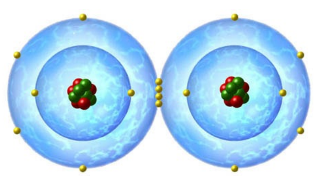

THE FOUNDATION OF GREAT MINDS
SINCE 2737 BC

Ch12

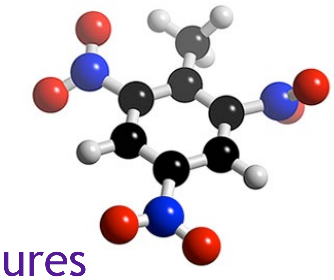
Chemical Bonds

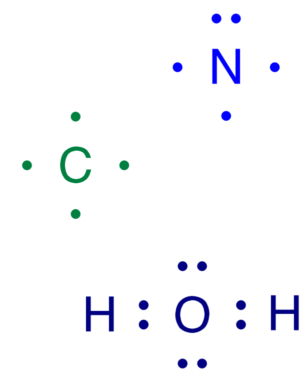
- Atoms to Molecules
  - Composition,
    Connectivity & Shape
  - Bonding (connectivity)
    - Metallic, Ionic & Covalent
- Lewis Symbols
  - Dots for valence Electrons
  - The octet rule
    - Cations
    - Anions
- Ionic Bonds
- Covalent Bonds
  - Bonding Pairs
    - Lone Pairs
  - Multiple Bonds

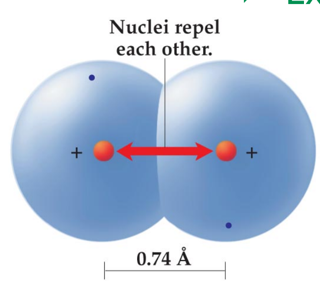


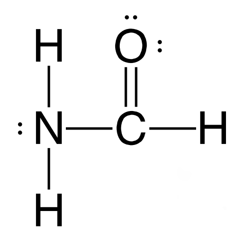


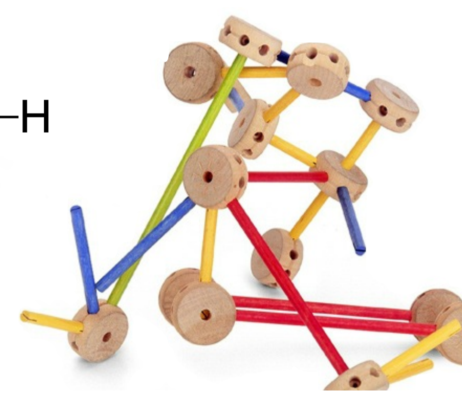
- Polar Covalent Bonds
  - Bond Dipoles
  - Electronegativity Scale
- How to Create Lewis Structures
  - Five Steps.
    - Take stock.
    - Draw a skeleton.
    - Distribute Electrons.
    - Push Electrons.
    - Evaluate Result.
  - Formal Charge
    - Resonance
    - Exceptions to the Octet Rule











A model for understanding connectivity.

Composition

(What's in it.)

CCl_4

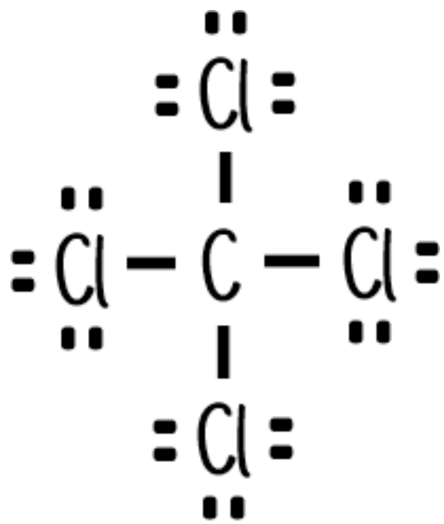
1 Carbon
4 Chlorine

Chemical Symbols

Molecular Formula

Connectivity

(What's connected to what.)



Lewis Dot Structure

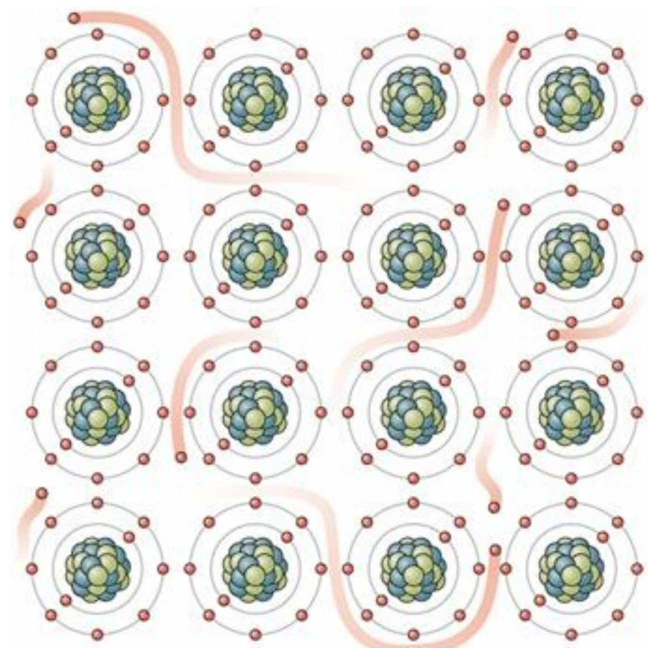
Shape

(Bond Angles & Distances)

(coming next)

Chemical Bonds

- Metallic Bonding:
  - In bulk metals (Fe, Au, Co) electrons break off and float between the atoms.
  - These free flowing electrons make metals extremely good conductors of electricity.
  - Metal atoms pull on the electrons flowing between them causing the mass to stick together.



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  - These free flowing electrons make metals extremely good conductors of electricity.
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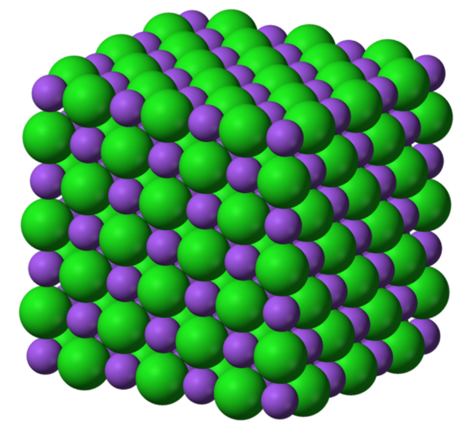
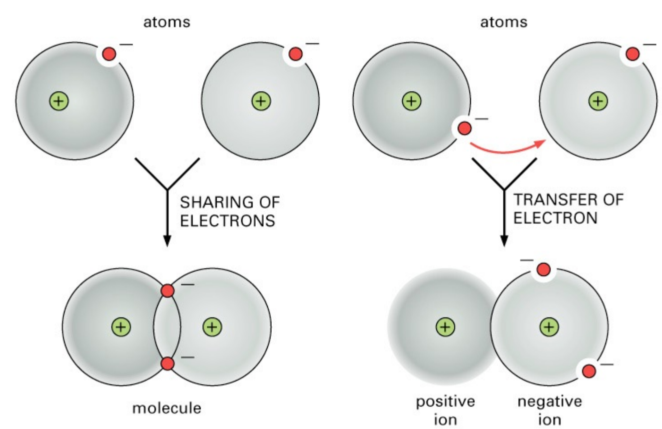
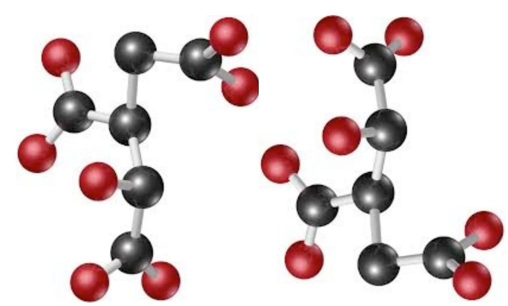
- Ionic Bonding:
  - In mixtures of metals and non-metals electrons break off from metals and are captured by non-metals.
  - This creates positively and negatively charged particles.
  - These ions clump together in simple, large complexes.
  - Ionic bonds are extremely strong.
- Covalent Bonding:
  - Nonmetals pull on each others electrons.
  - If neither non-metal pulls hard enough to remove the electron from the other, the two end up sharing a pair of electrons.
  - The shared electrons are localized between two atoms, creating bond between those atoms.







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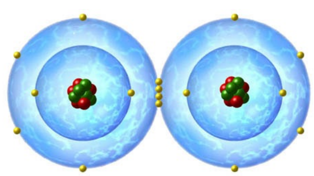

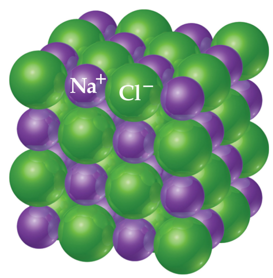

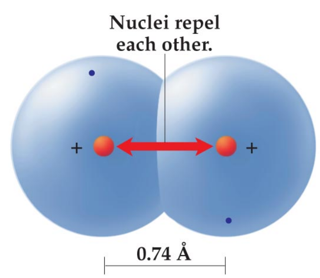

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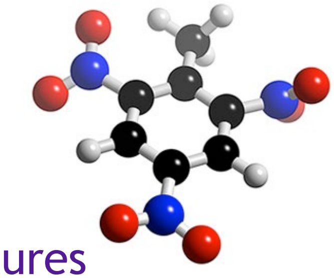
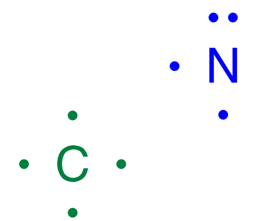
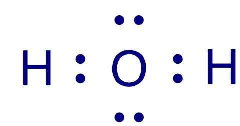
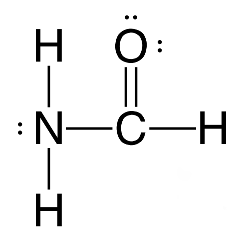
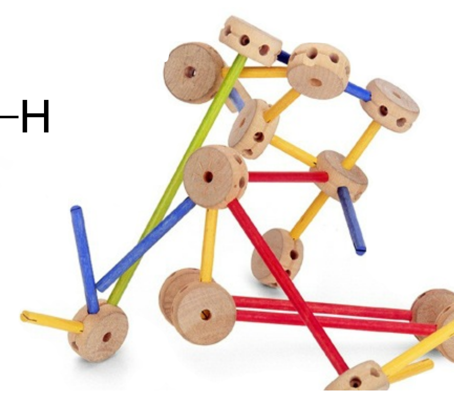




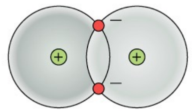






Gilbert N. Lewis

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



- Coined the term Photon

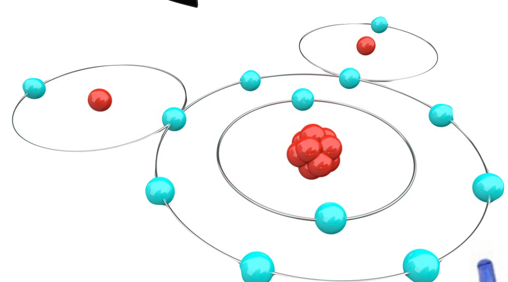
  - Although Planck and Einstein advanced the concept of quanta, Einstein did not use the word photon in his early writings and as far as my reading goes, he never did. The word "photon" originated from Gilbert N. Lewis years after Einstein's photoelectric paper and appeared in a letter to the editor of 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)

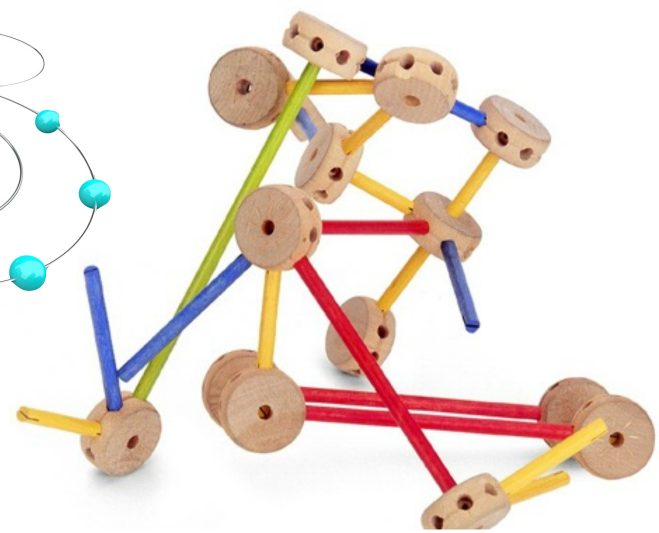
- Formalized the electron pair theory of Acids & Bases which is why we call them “Lewis Acids”

- 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



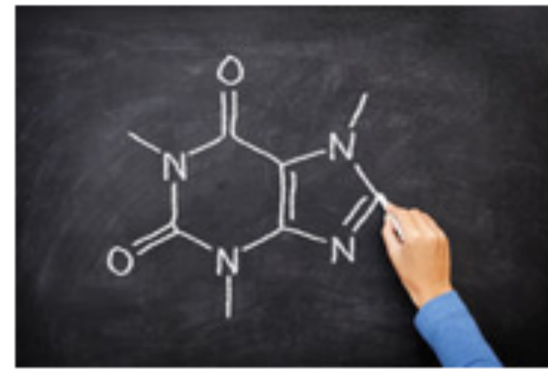
- Nominated for a nobel prize 35 times

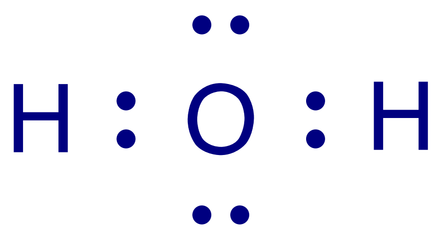
  (Mahatma Gandhi was only nominated 5 times)
  - *He never received one.*
- Lewis was found dead at his lab bench at UC Berkeley in 1946, his death may have been due to poisoning from chemicals in his experiment. The coroner listed it as a heart attack.
- Developed Valence Shell Notation
  - more commonly known as Lewis Dot Structures

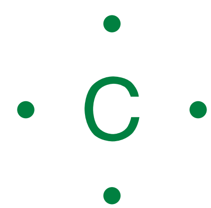


It starts with Lewis Symbols

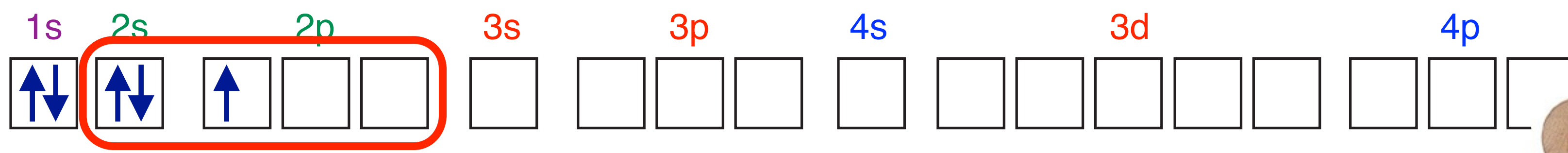
- Lewis notation is how we described the connectivity of all covalent compounds (molecules).
- It's how we show the difference between compounds that have the same composition (molecular formula).
- Lewis notation starts with understanding the Lewis symbols for each atom or ion.
- Symbols that communicate the valence structure of the electronic configuration of those particles.







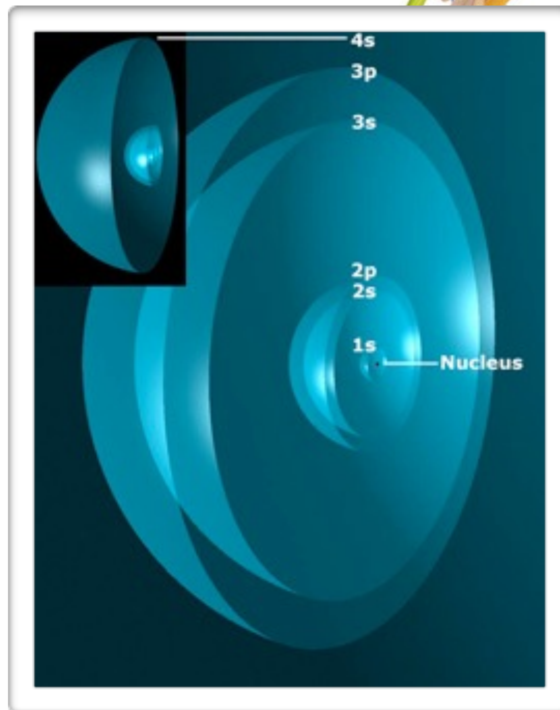
Lewis Symbols

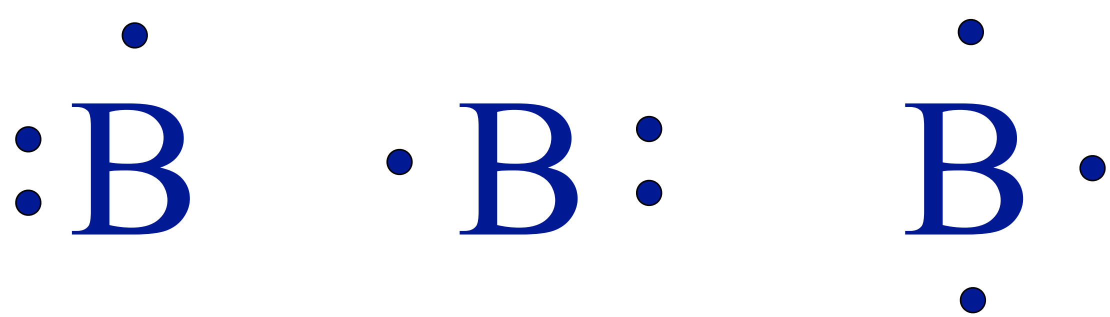


- The electrons involved in bonding are called valence electrons.
- Valence electrons are found in the incomplete, outermost shell of an atom. The valence shell.
- As a pictorial understanding of where the electrons are in an atom, we represent the electrons as dots around the symbol for the element.
- The number of valence electrons available for bonding are indicated by unpaired dots.
- We generally place the electrons on four sides of a square around the element's symbol.

B

- These symbols are called Lewis symbols or Lewis electron-dot symbols.





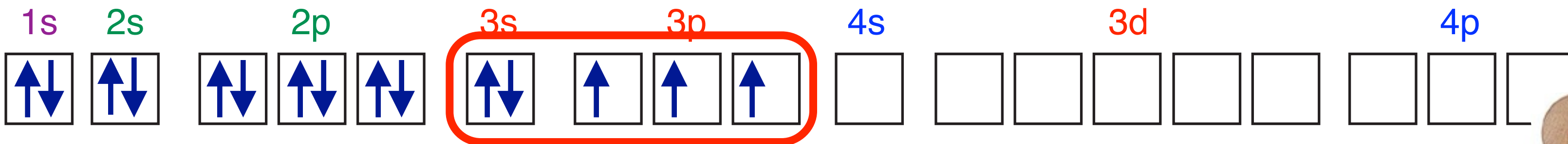
ground state

excited state

$1s^2 2s^2 2p^1$

5 electrons
3 valence electrons

Lewis Symbols



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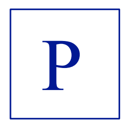

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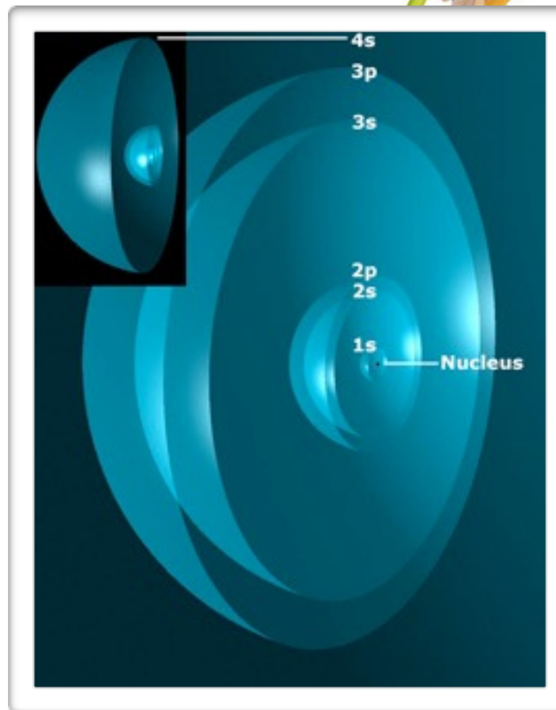
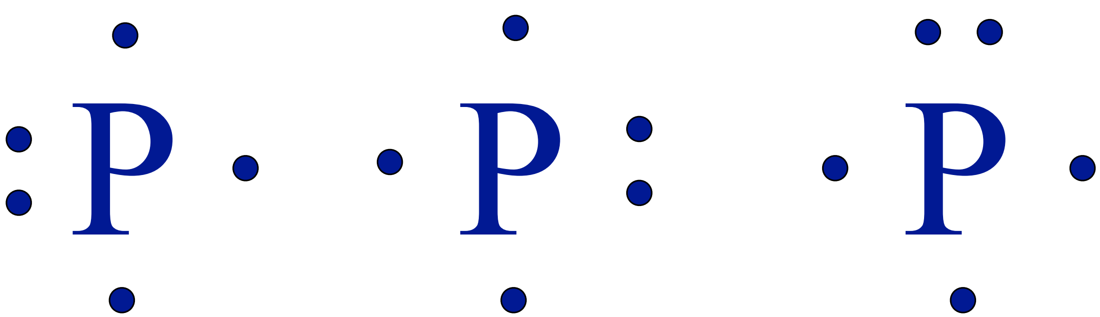




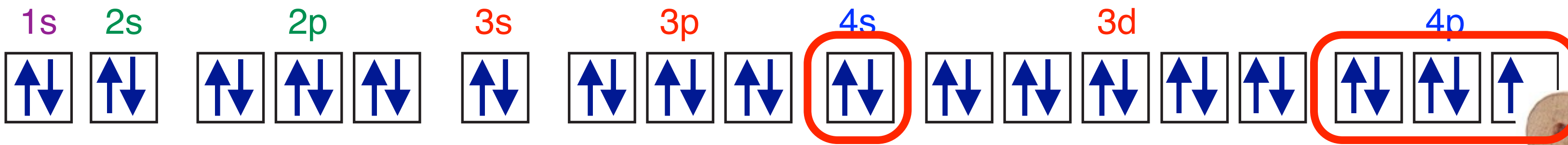
ground state

$1s^2 2s^2 2p^6 2s^2 2p^3$

15 electrons

5 valence electrons

Lewis Symbols



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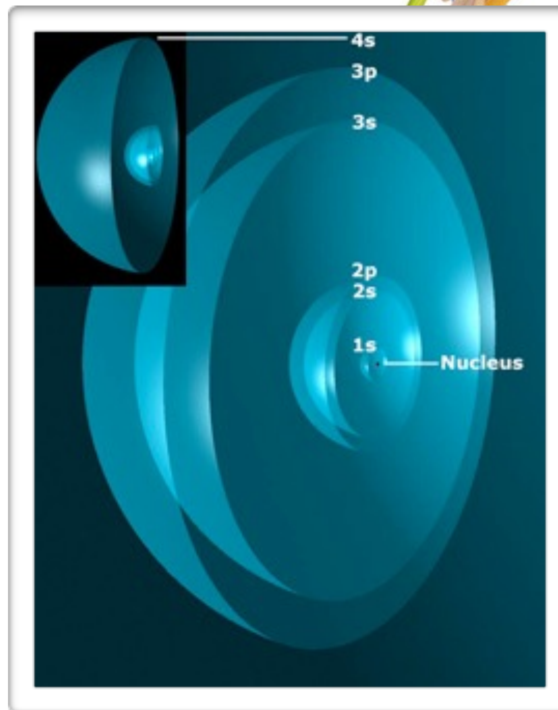
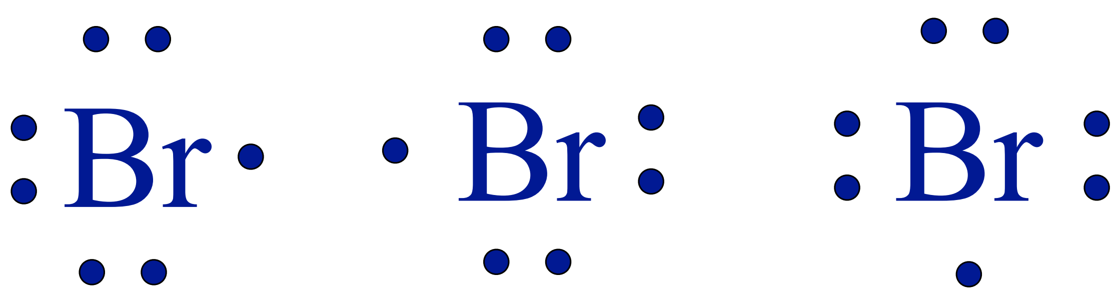
Br





ground state

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$

35 electrons

7 valence electrons

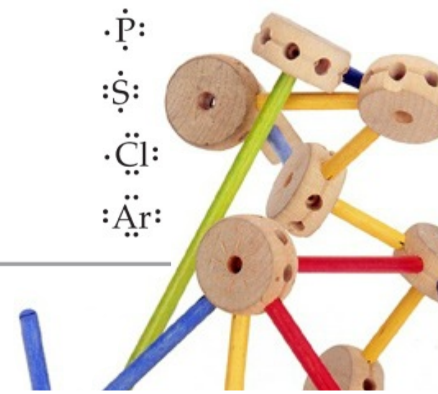
Lewis Symbols

	1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	9	10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	113	114	115	116		118

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

Metals
Metalloids
Nonmetals

Element	Electron Configuration	Lewis Symbol
Li	[He]$2s^1$	Li·
Be	[He]$2s^2$	·Be·
B	[He]$2s^22p^1$	·Ḃ·
C	[He]$2s^22p^2$	·Ċ· (4 dots)
N	[He]$2s^22p^3$	·N̈:
O	[He]$2s^22p^4$	:Ö:
F	[He]$2s^22p^5$	·F̈:
Ne	[He]$2s^22p^6$	:N̈e:
Na	[Ne]$3s^1$	Na·
Mg	[Ne]$3s^2$	·Mg·
Al	[Ne]$3s^23p^1$	·Ȧl·
Si	[Ne]$3s^23p^2$	·Ṡi·
P	[Ne]$3s^23p^3$	·P̈:
S	[Ne]$3s^23p^4$	:S̈:
Cl	[Ne]$3s^23p^5$	·C̈l:
Ar	[Ne]$3s^23p^6$	:Är:



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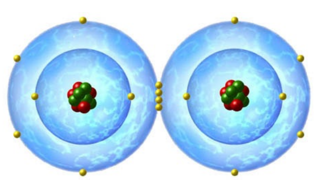

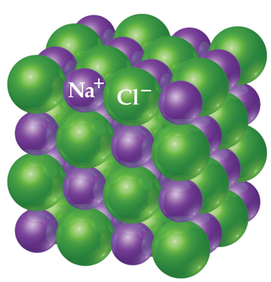

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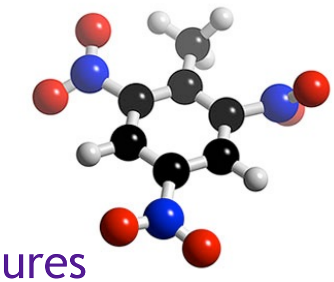
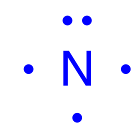
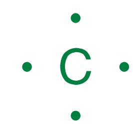
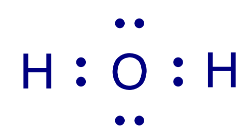
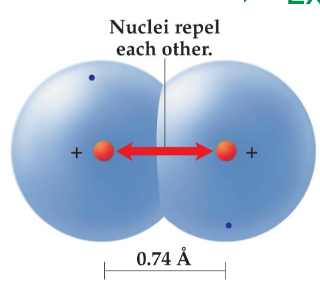
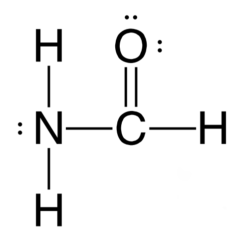


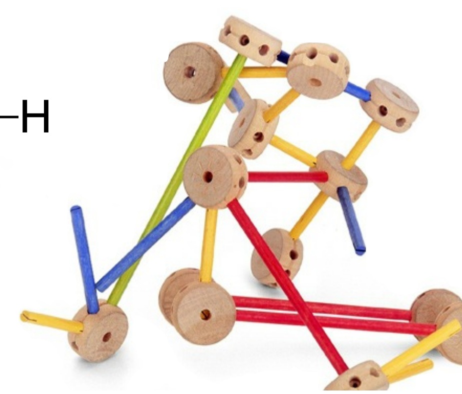




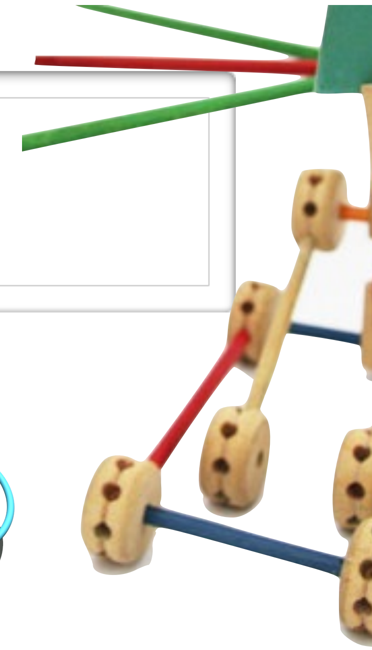


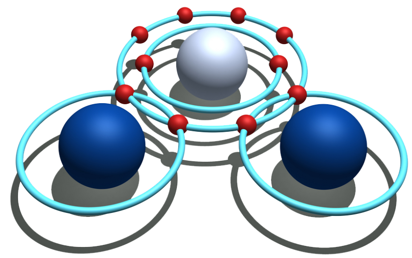




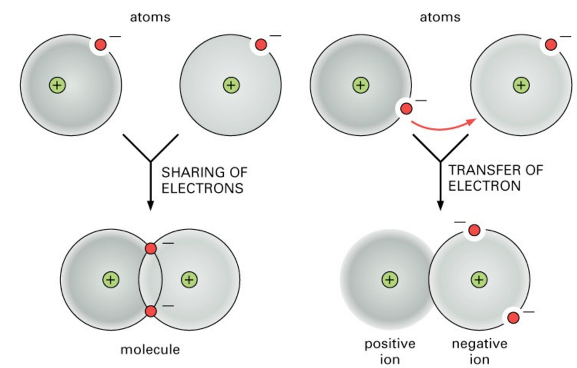


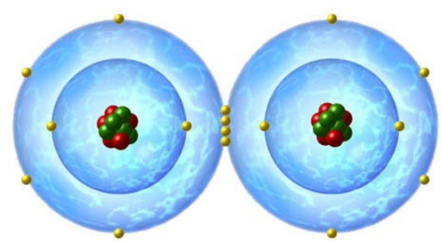
The Octet Rule

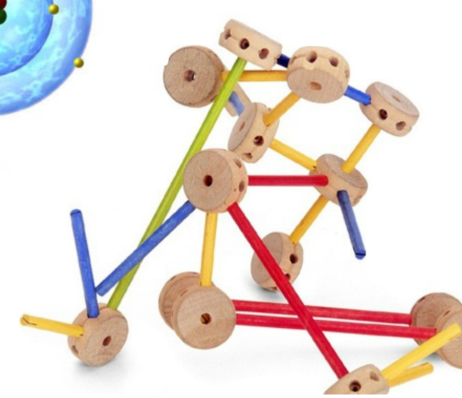




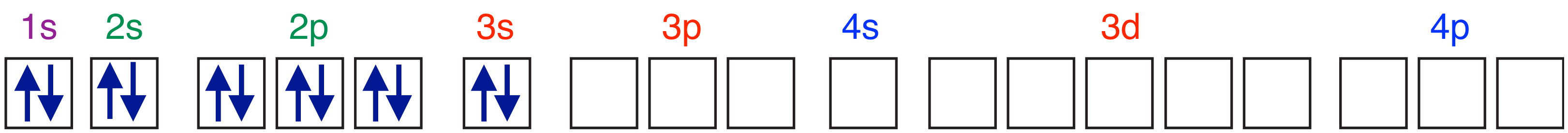
- A full valence shell is a plateau in energy.
  - There's a considerable gain in energy by reaching a full shell.
  - There's little gain in trying to add more electrons.
- The valence shell for all main group atoms (for this class we will say all atoms) have between 1-8 electrons
- The octet rule:
  - 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.
      - We'll talk about this more later in this chapter.
    - 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







Lewis Symbols - Cations

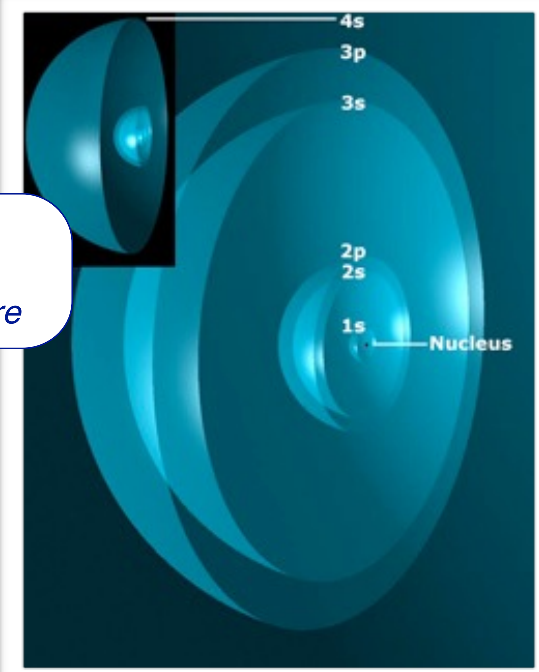


- For cations, start with the lewis dot symbol of the neutral element and remove the appropriate electrons.
- Then put the corresponding charge on the symbol.

$$\bullet\mathrm{Mg}\bullet \longrightarrow \mathrm{Mg}^{2+}$$

$1s^2 2s^2 2p^6 \underline{3s^2}$ $\qquad$ $1s^2 2s^2 2p^6$

for **most** cations:
8 valence electrons
but no dots in structure



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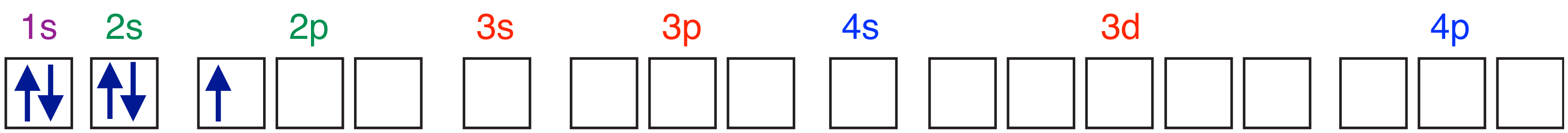


- For cations, start with the lewis dot symbol of the neutral element and remove the appropriate electrons.
- Then put the corresponding charge on the symbol.

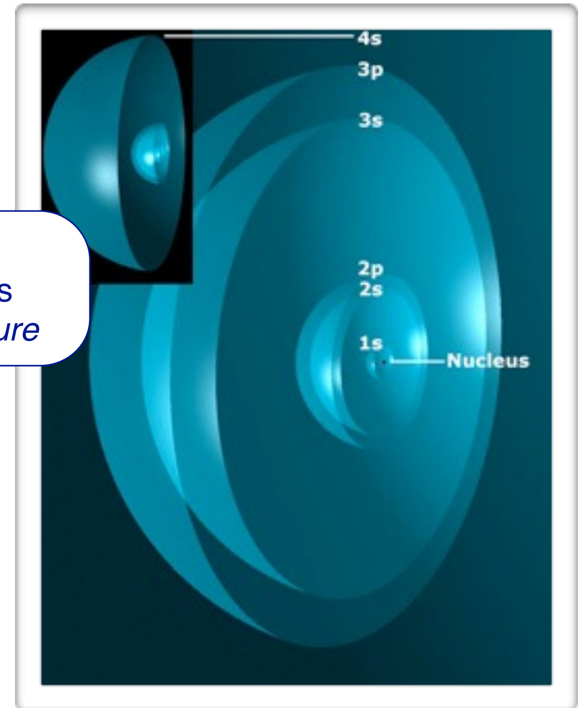
•Mg• → Mg^{2+}

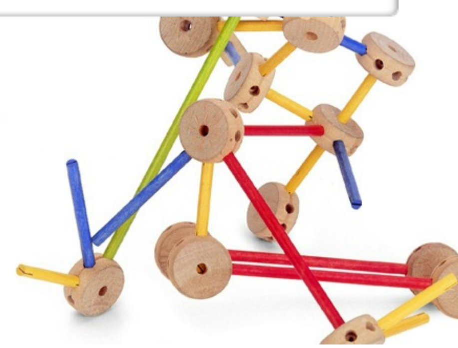
$1s^2 2s^2 2p^6 \underline{3s^2}$ → $1s^2 2s^2 2p^6$

:B• → B^{3+}

$1s^2 \underline{2s^2 2p^1}$ → $1s^2$

for **most** cations:
8 valence electrons
but no dots in structure





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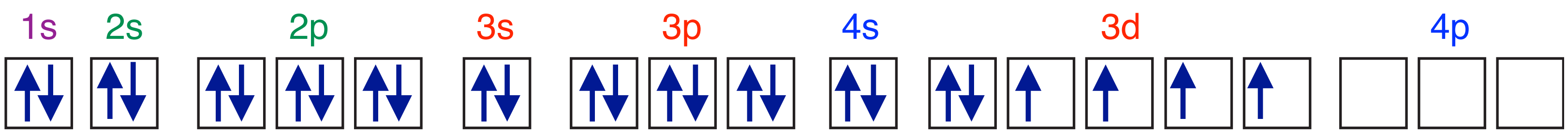
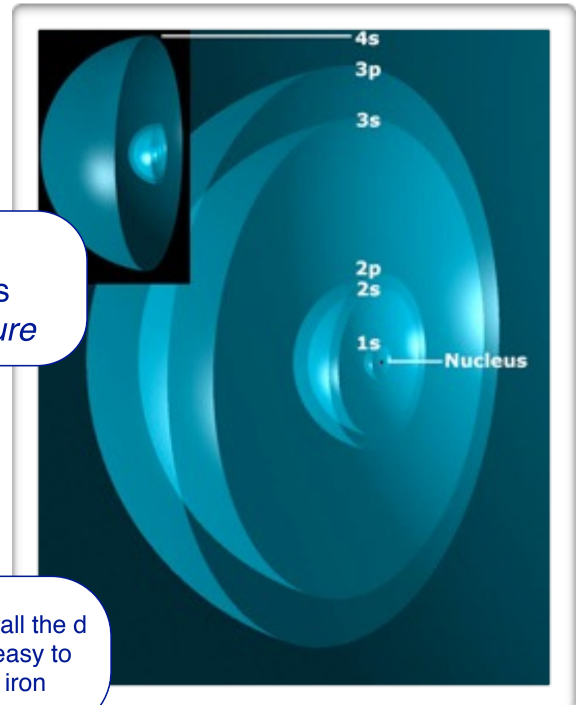


- For cations, start with the lewis dot symbol of the neutral element and remove the appropriate electrons.
- Then put the corresponding charge on the symbol.



for **most** cations:
8 valence electrons
but no dots in structure

$\cdot Mg \cdot \longrightarrow Mg^{2+}$

$1s^2 2s^2 2p^6 \underline{3s^2}$ → $1s^2 2s^2 2p^6$

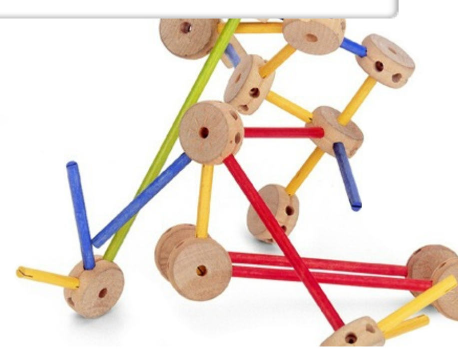
$:B\cdot \longrightarrow B^{3+}$

$1s^2 \underline{2s^2 2p^1}$ → $1s^2$

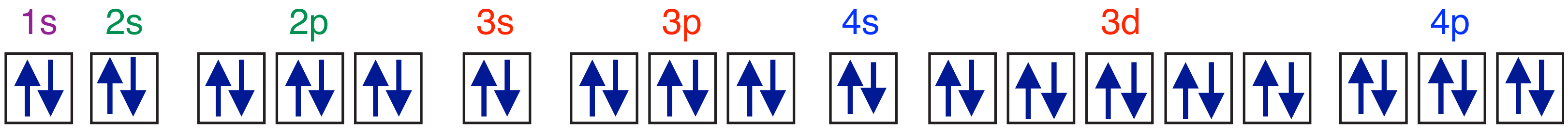
the stabilization from having all the d orbitals half filled makes it easy to pull a third electron off of iron

$\cdot Fe \cdot \longrightarrow Fe^{2+}$ Fe^{3+}

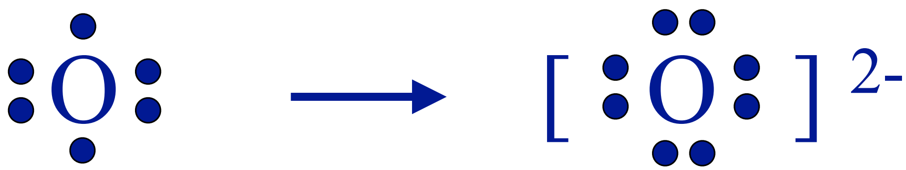
$1s^2 2s^2 2p^6 3s^2 3p^6 \underline{4s^2} 3d^6$ → $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$ $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$



Lewis Symbols - Anions

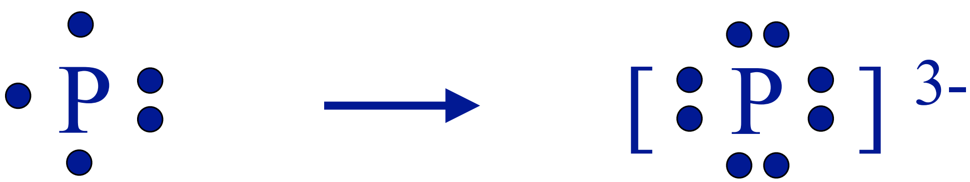


- For anions, start with the lewis dot symbol of the neutral element and add the appropriate electrons.
- Put brackets around the symbol *to be clear those extra electrons belong to it*.
- Then put the corresponding charge on the symbol — <u>outside the bracket</u>.

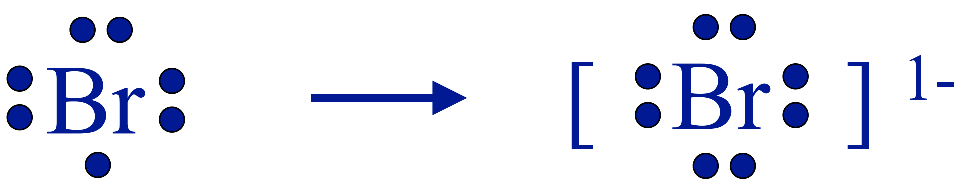


$1s^2 2s^2 2p^4$ $\quad$ $1s^2 2s^2 2p^6$

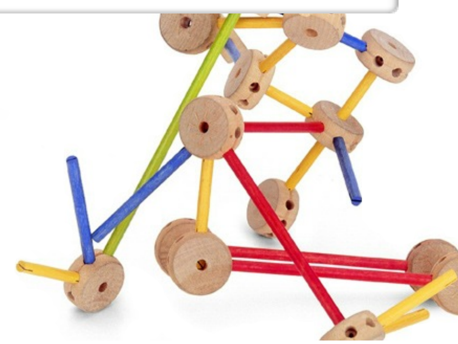
for **<u>most</u>** anions:
8 valence electrons
8 dots in structure
don't forget the brackets!



$1s^2 2s^2 2p^6 3s^2 3p^3$ $\quad$ $1s^2 2s^2 2p^6 3s^2 3p^6$



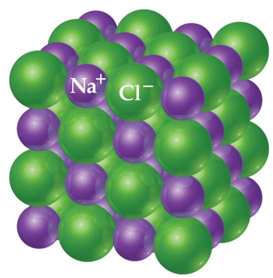
$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$ $\quad$ $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

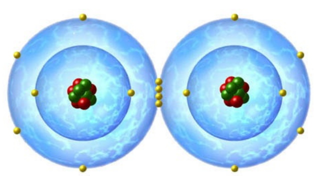


Ch12

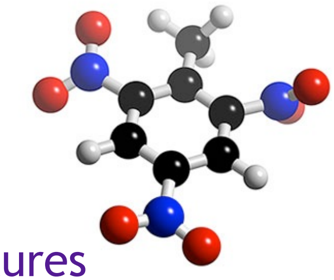
Chemical Bonds

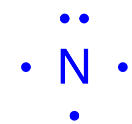
- Atoms to Molecules
  - Composition, Connectivity & Shape
  - Bonding (connectivity)
    - Metallic, Ionic & Covalent
- Lewis Symbols
  - Dots for valence Electrons
  - The octet rule
    - Cations
    - Anions
- Ionic Bonds
- Covalent Bonds
  - Bonding Pairs
    - Lone Pairs
  - Multiple Bonds

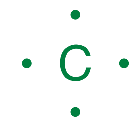


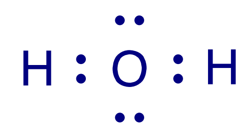


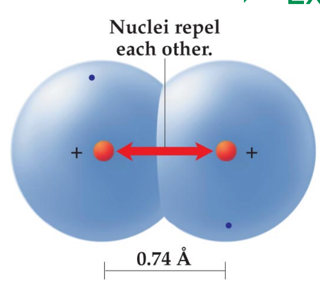
- Polar Covalent Bonds
  - Bond Dipoles
  - Electronegativity Scale
- How to Create Lewis Structures
  - Five Steps.
    - Take stock.
    - Draw a skeleton.
    - Distribute Electrons.
    - Push Electrons.
    - Evaluate Result.
  - Formal Charge
    - Resonance
    - Exceptions to the Octet Rule

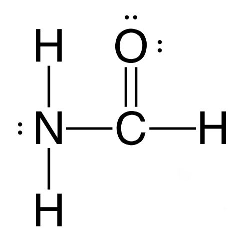






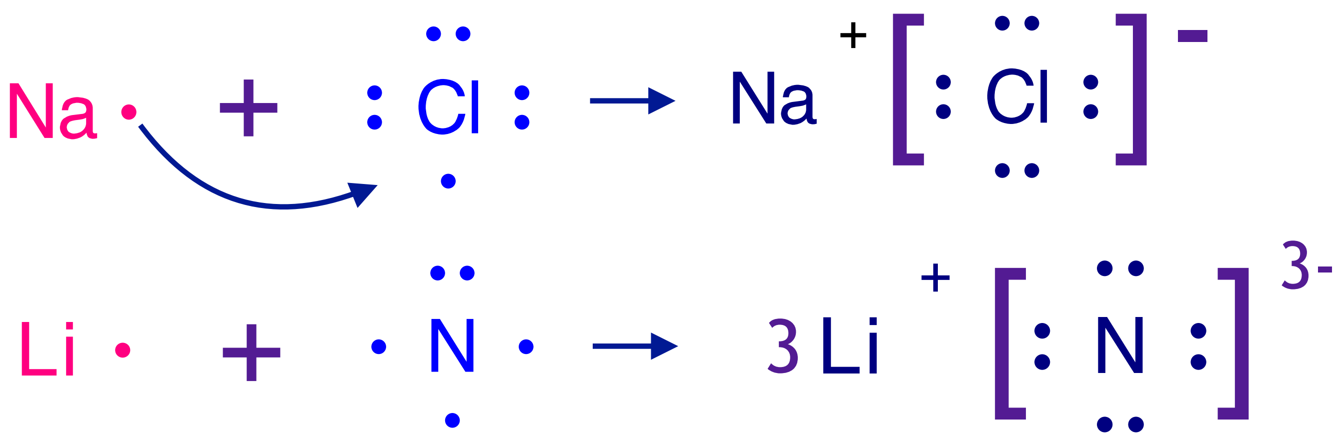






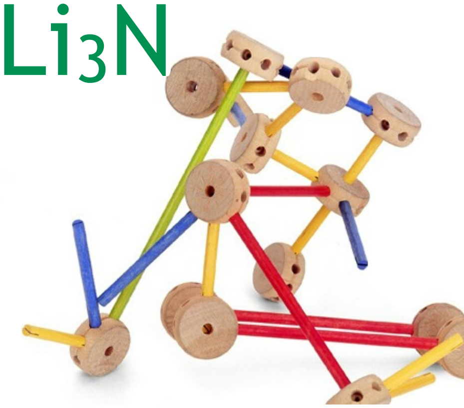
Ionic Bonding

- 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



Ch12

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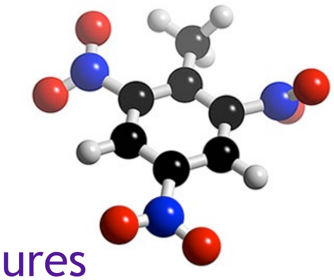
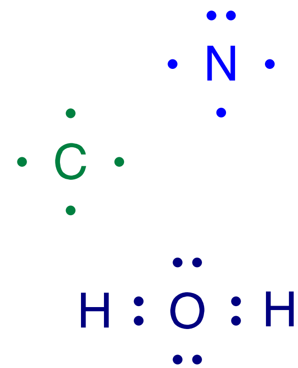
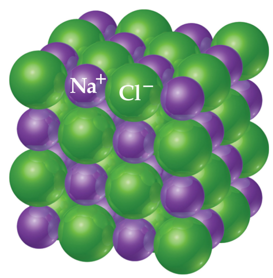
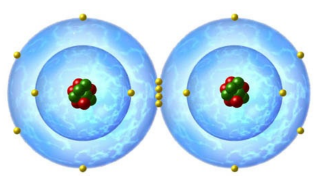
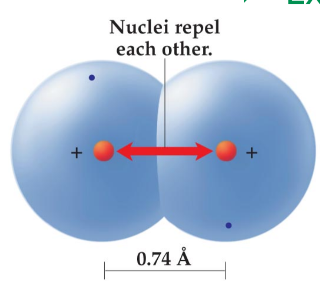
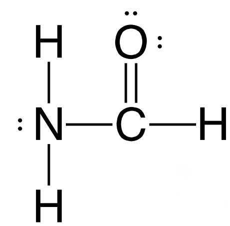


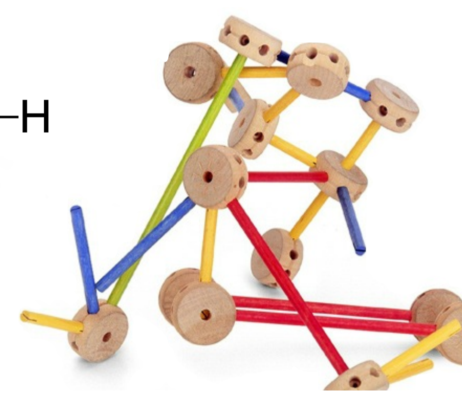






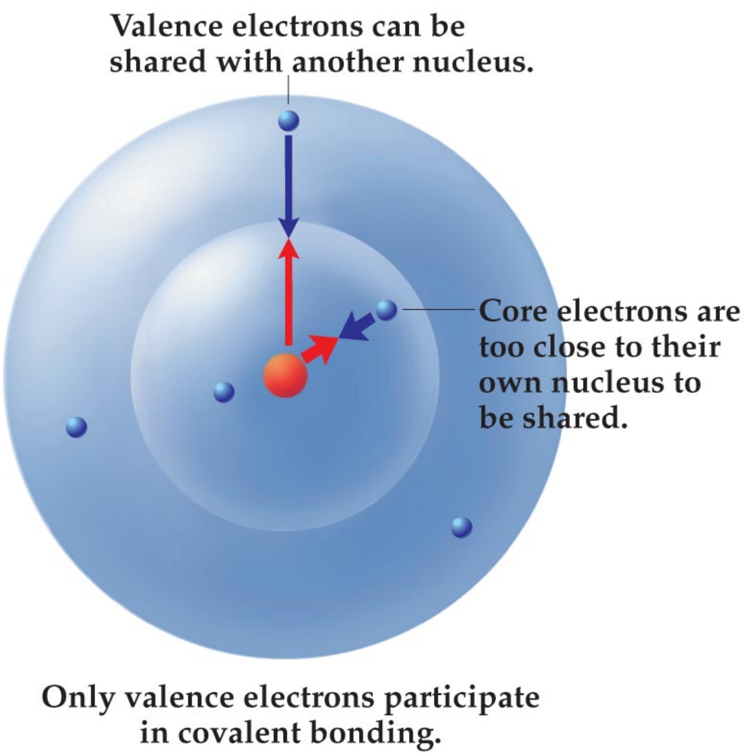


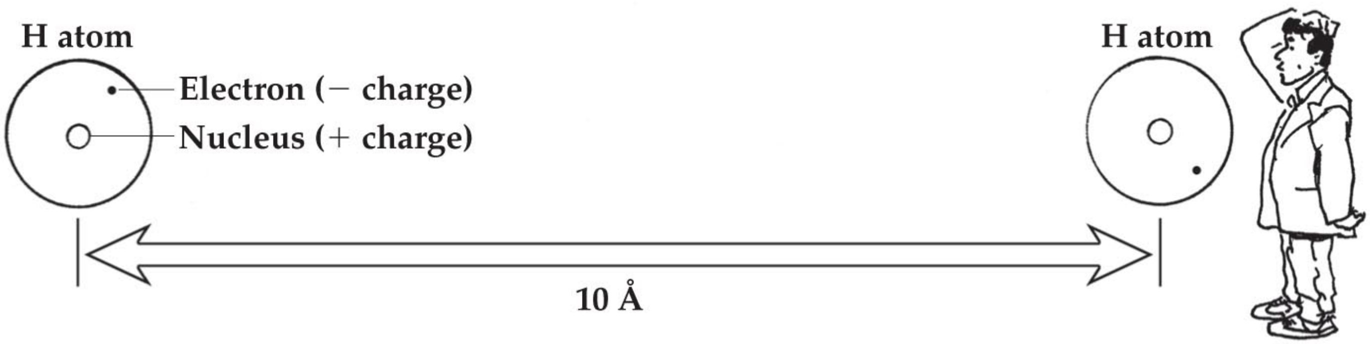




The Covalent Bond

- 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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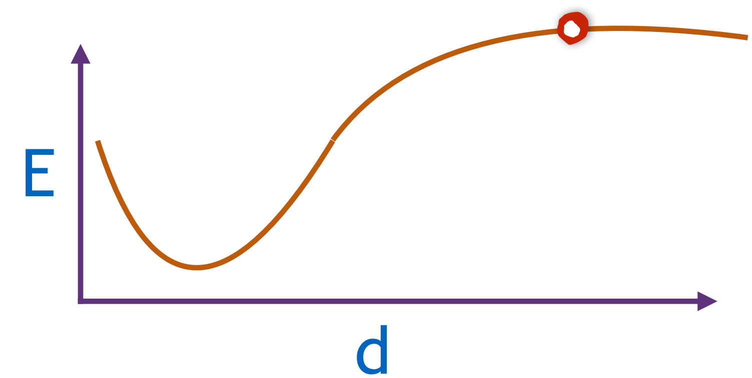

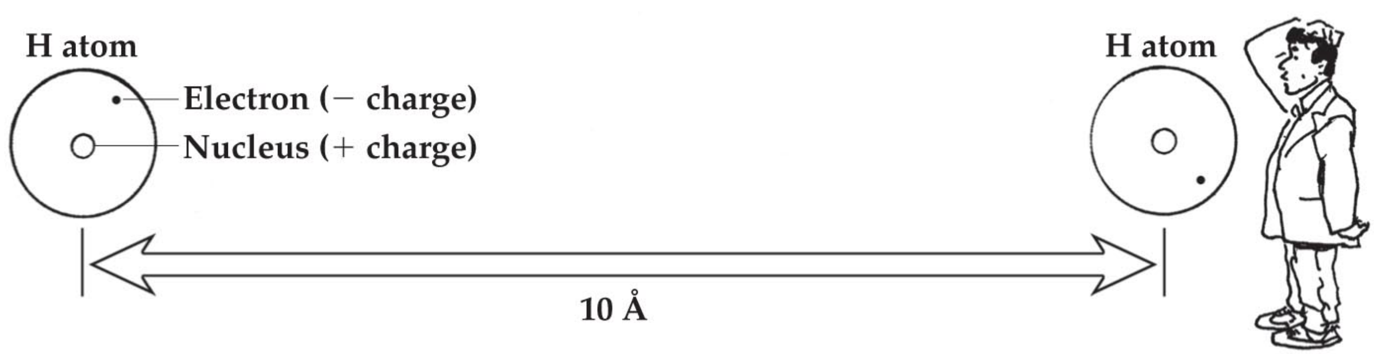

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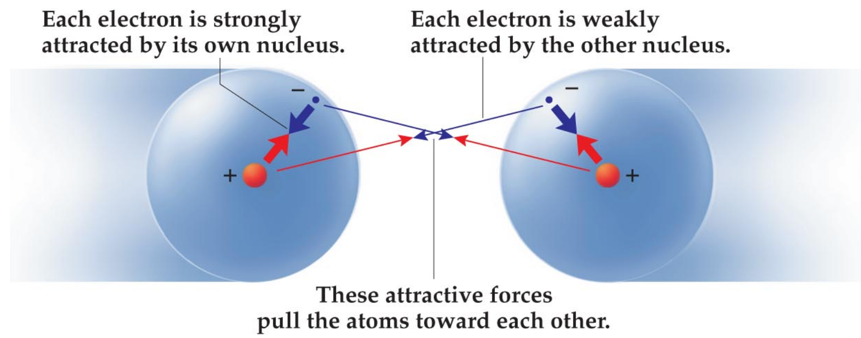

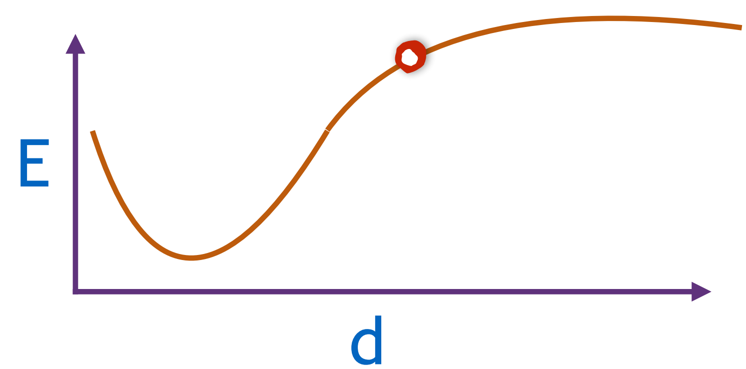

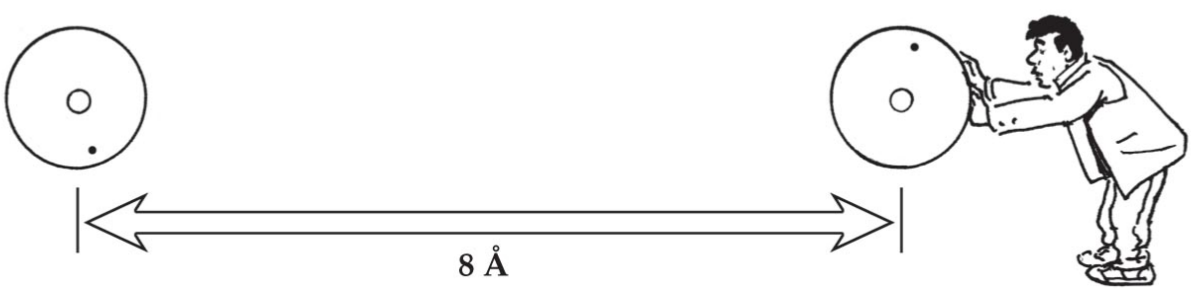

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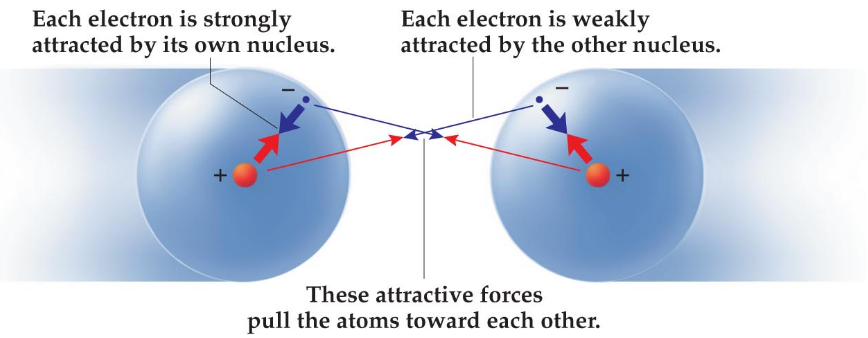

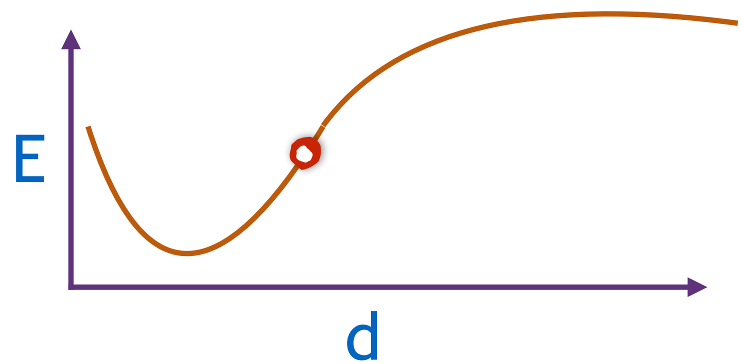

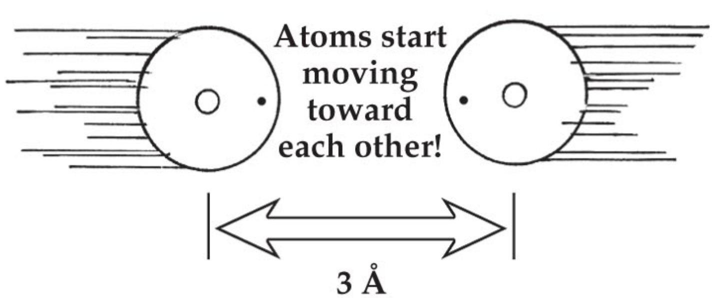

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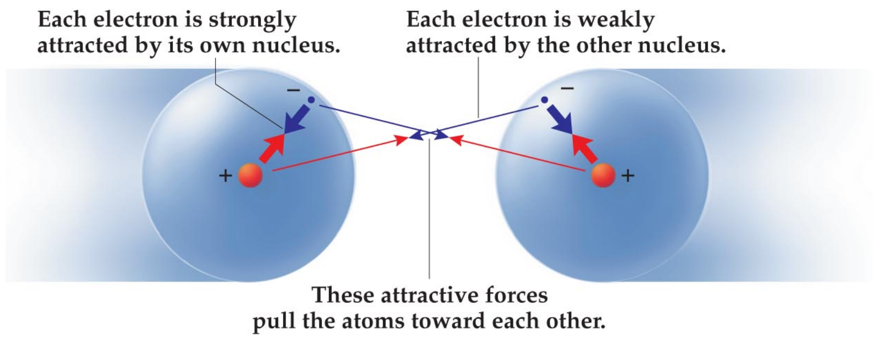

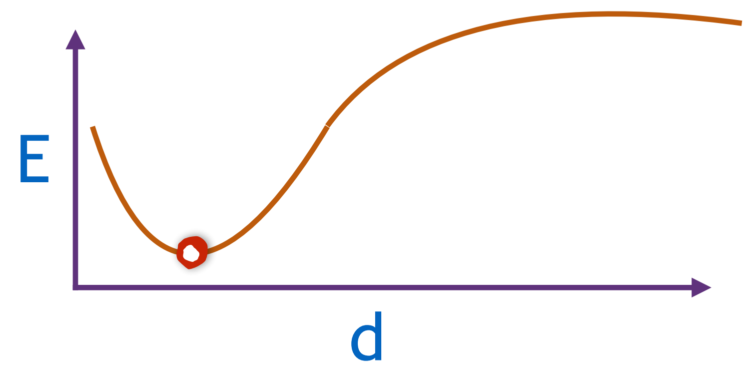

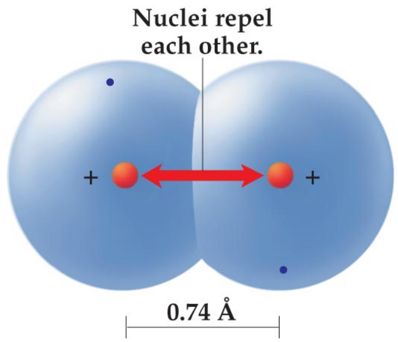

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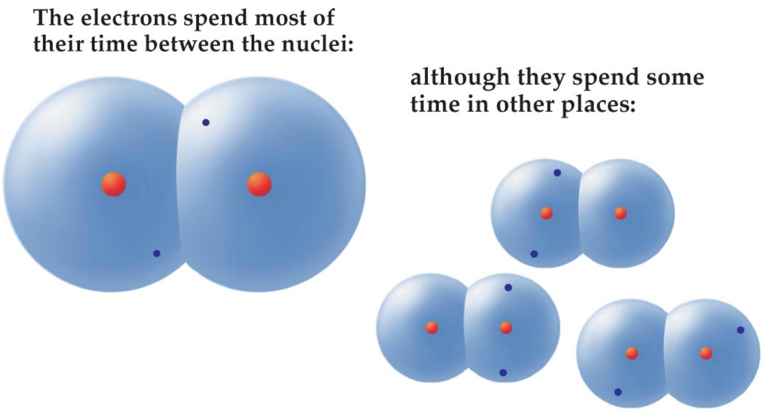

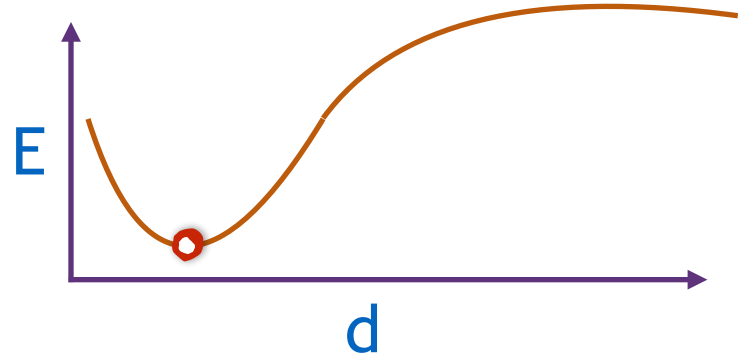

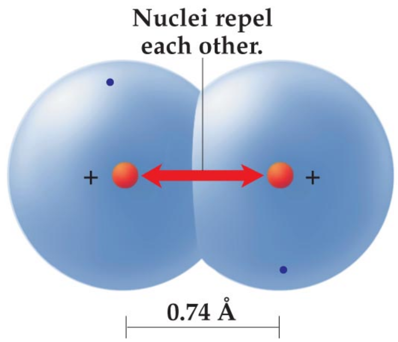

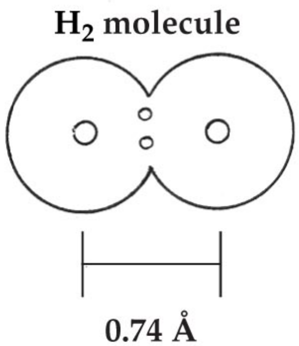

Chemical Bonds

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  - Composition, Connectivity & Shape
  - Bonding (connectivity)
    - Metallic, Ionic & Covalent
- Lewis Symbols
  - Dots for valence Electrons
  - The octet rule
    - Cations
    - Anions
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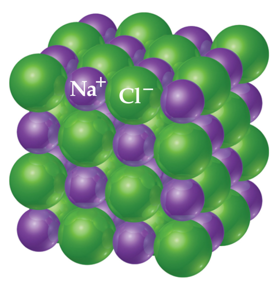
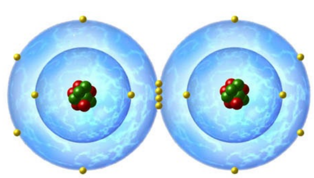
- Covalent Bonds
  - Bonding Pairs
    - Lone Pairs
  - Multiple Bonds





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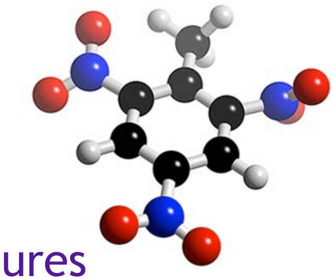
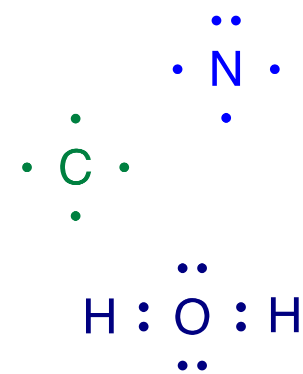
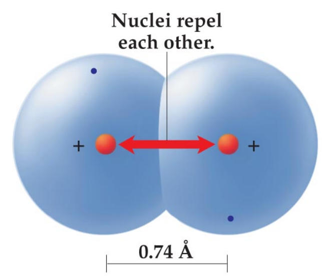
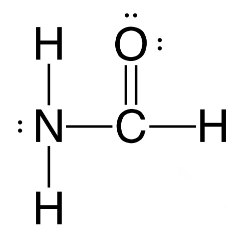
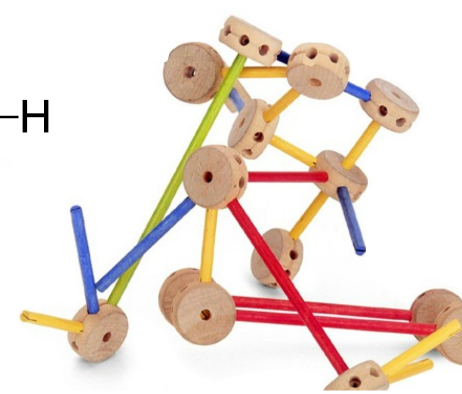




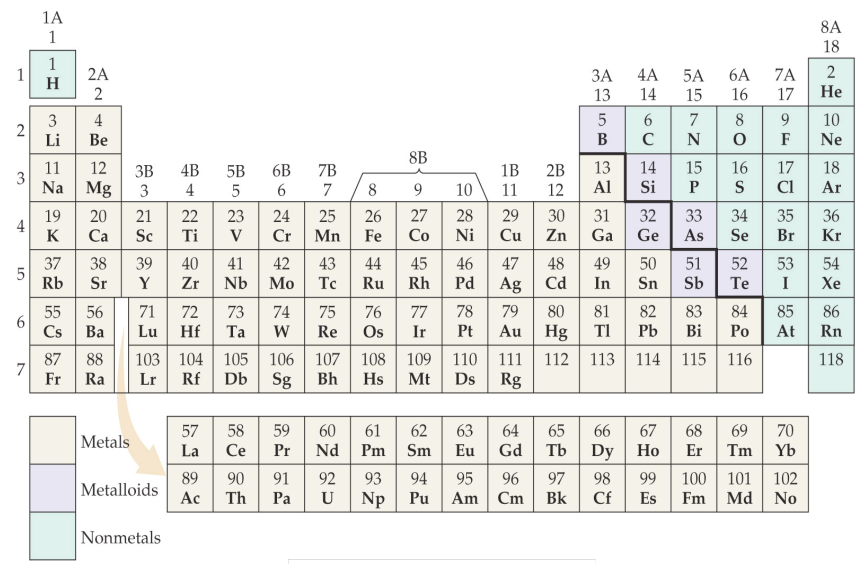


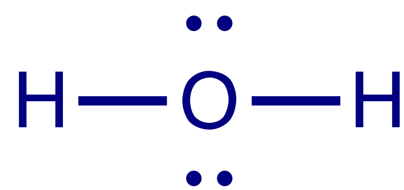


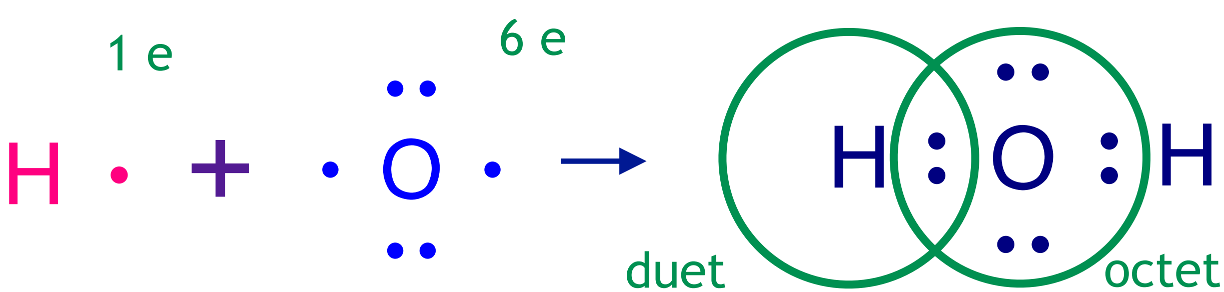


Lewis Molecular Structures

- Lewis symbols provide a simple way of visualizing and predicting covalent bonds.
- Atoms with less than a full valence entangle their orbitals to share electron pairs.
  - 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.
- Electron pairs involved in bonding are called bonding pairs.
  - Bonding pairs may be replaced with a single line.
- Main group elements can form one, two, or three covalent bonds.







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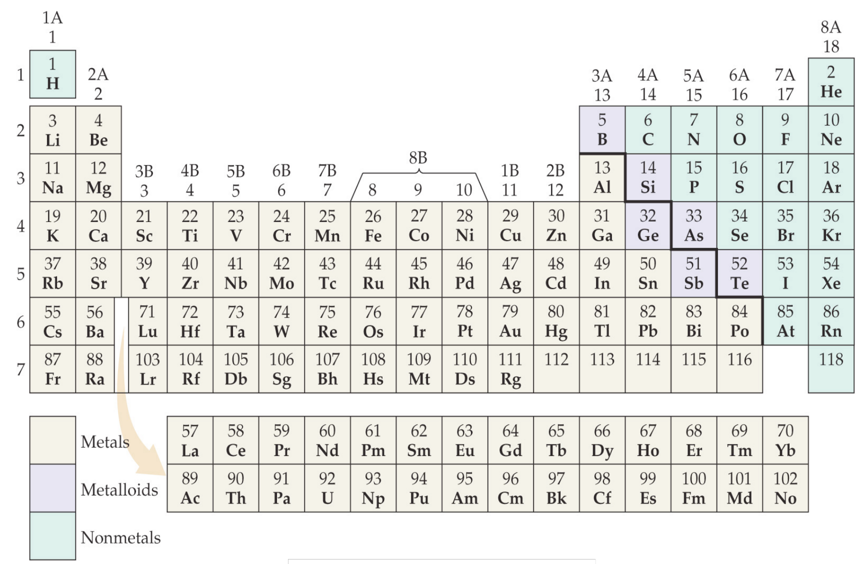

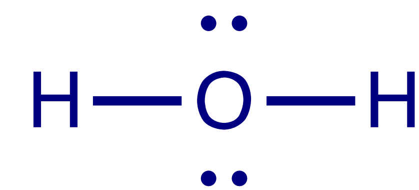

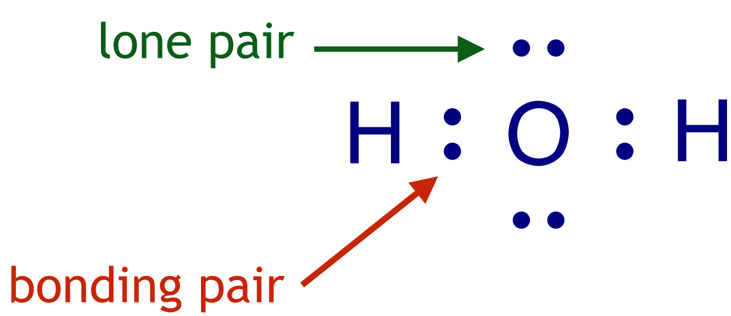

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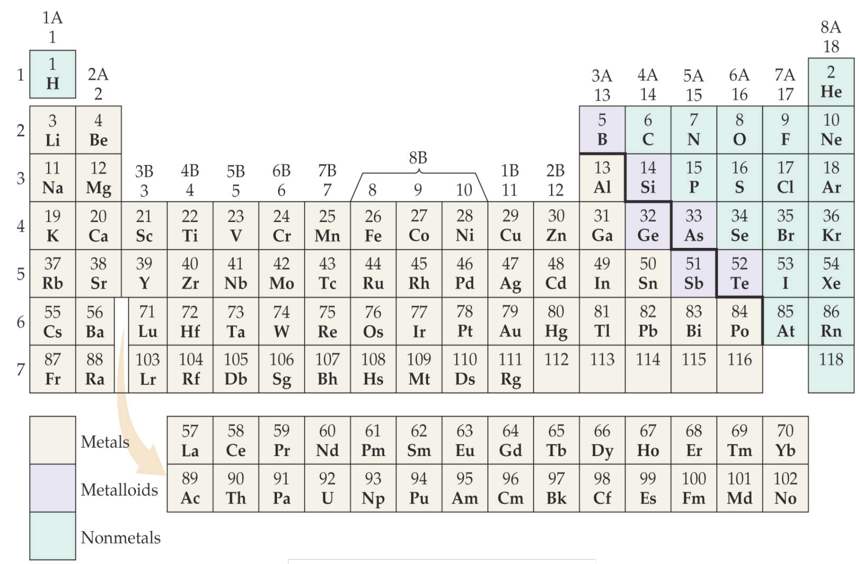

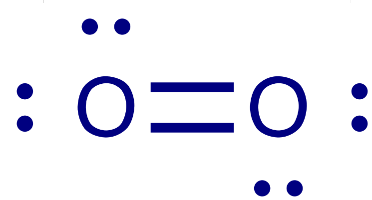

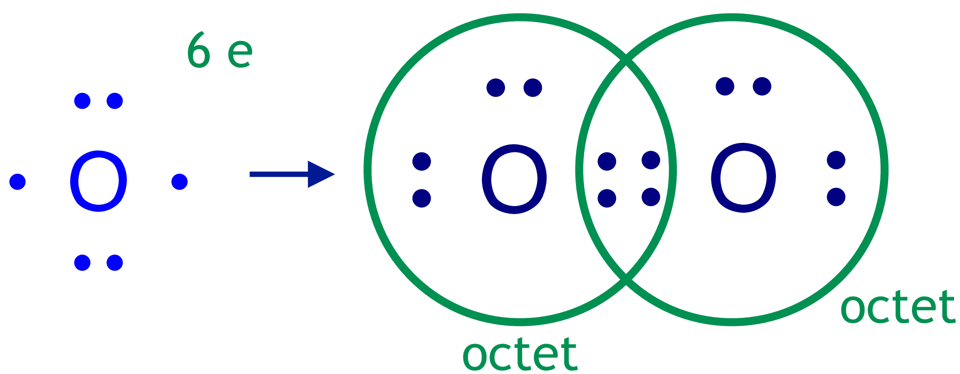

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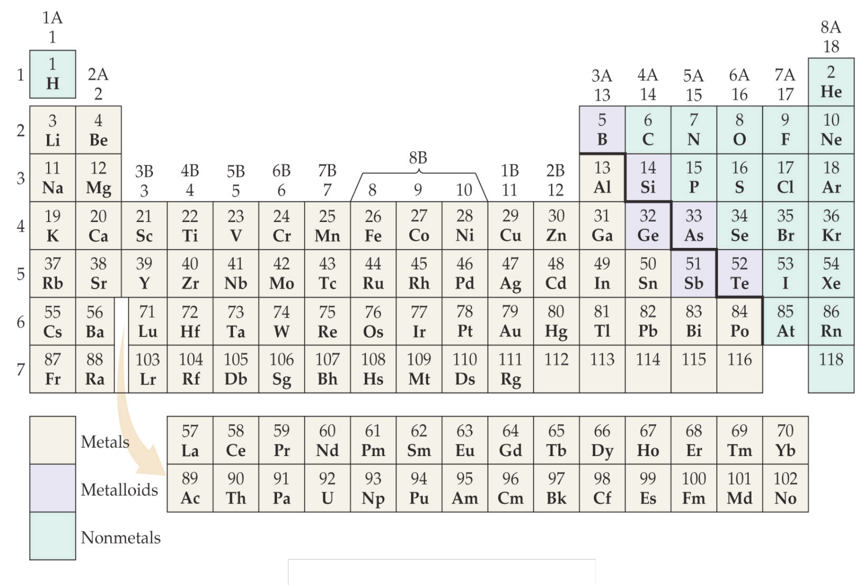

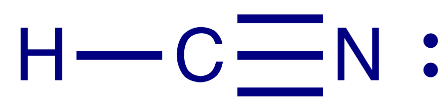

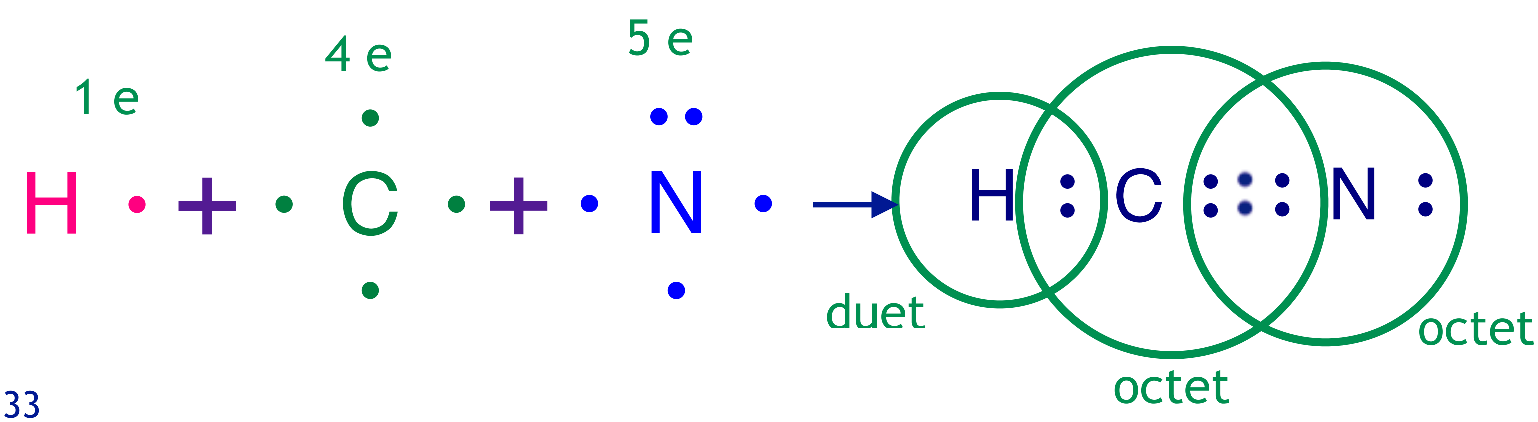

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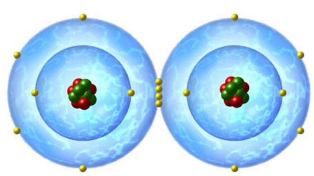

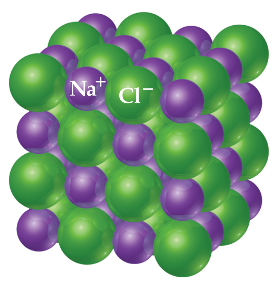

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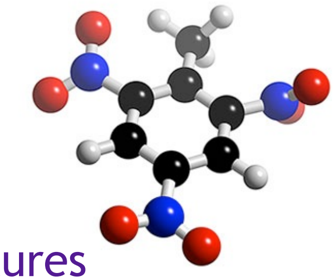
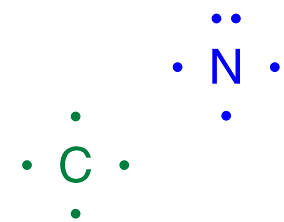
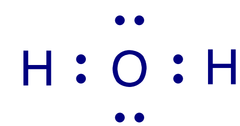
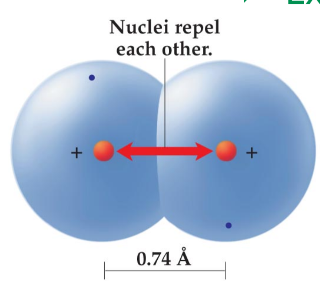
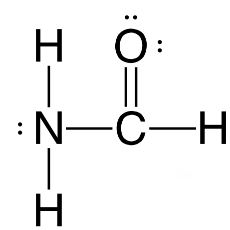
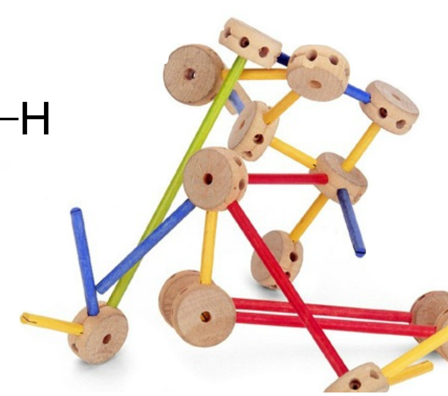






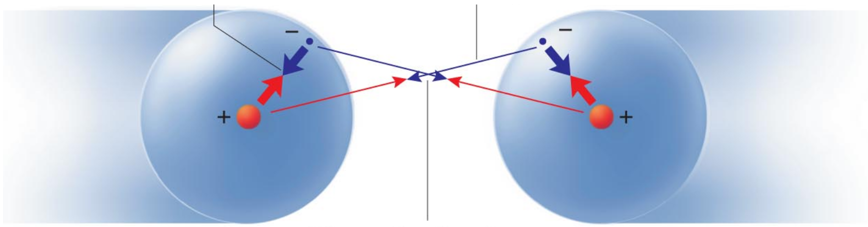


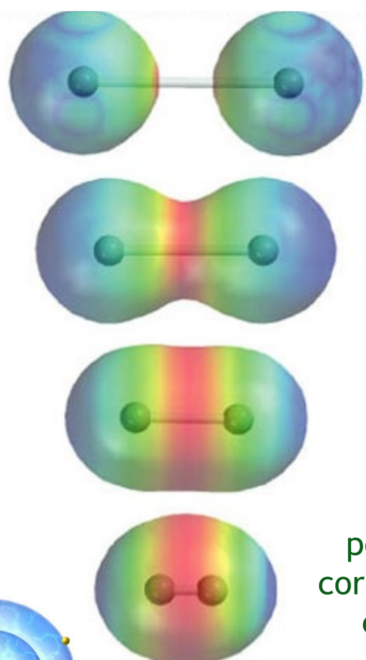




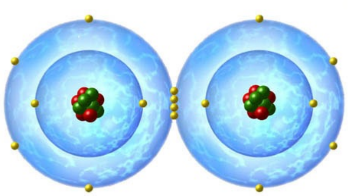
Covalent Bonds

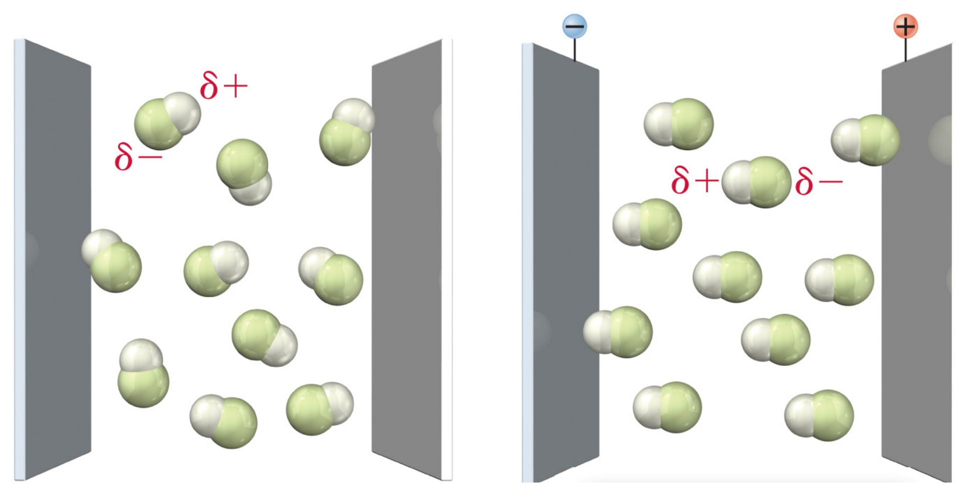
- Covalent Bonds are a result of atoms pulling on each others electrons.
- The atoms lock into a fixed distance from each other, entangling their orbitals.
- The shared electrons complete each atoms octet, making a stable combined arrangement of electrons.
- Some molecules placed in a electric field 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.



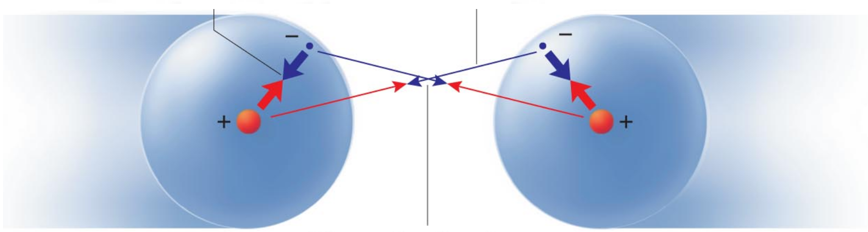


(in electrostatic potential maps red corresponds to greater electron density, blue indicates lesser density)

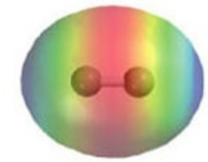


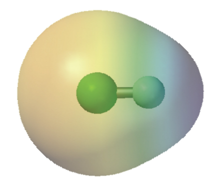


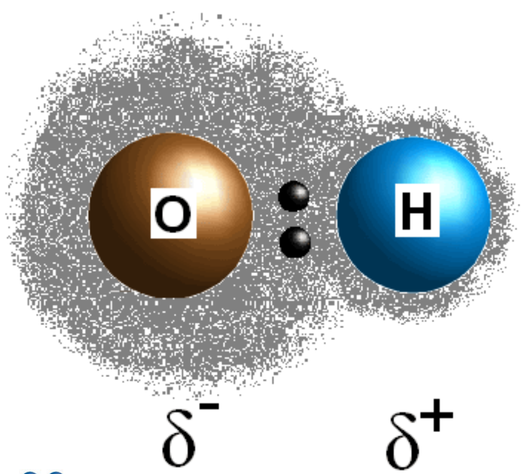
Polar Covalent Bonds

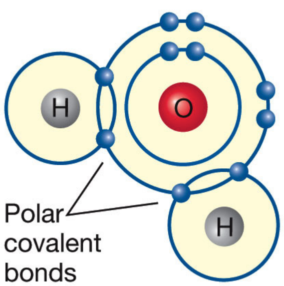


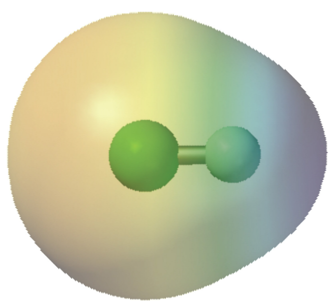
- Pure covalent bonds are symmetric.
  - Not all covalent bonds are pure.
- Sometimes one atom pulls stronger on the shared electrons than the other.
- Polar covalent bonds are covalent bonds with asymmetric sharing of the bonding pair.

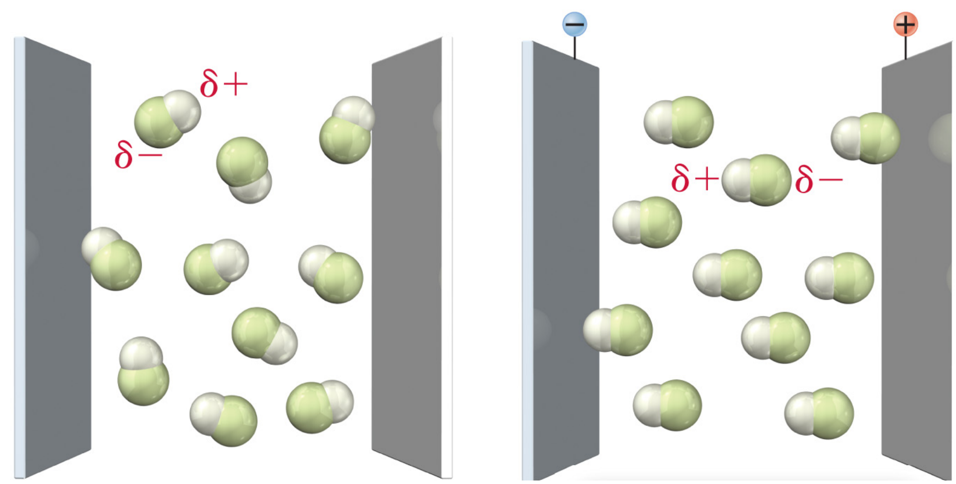










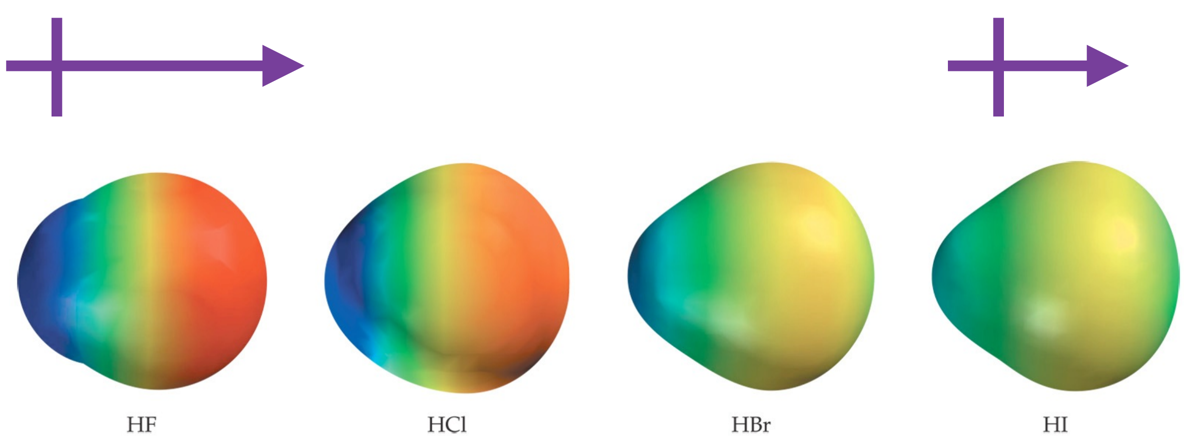


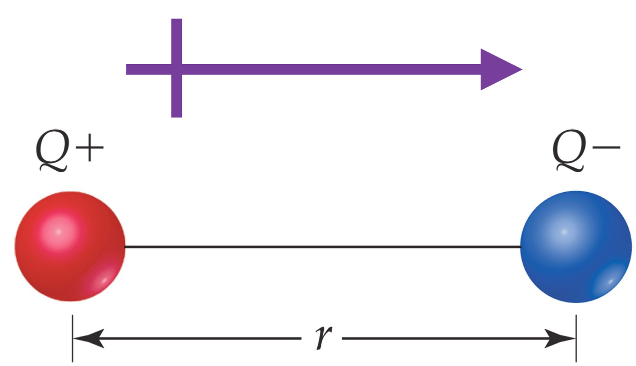
Bond Dipoles

- 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.





Ch12

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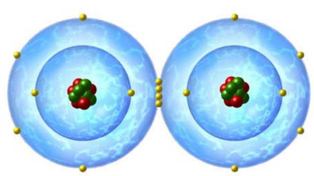

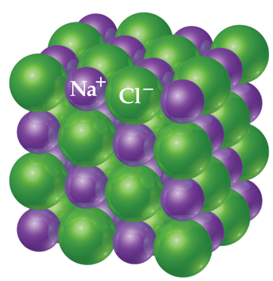

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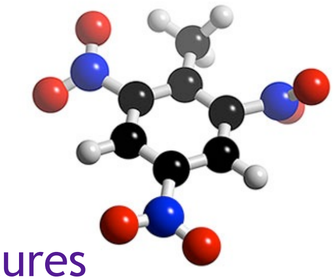
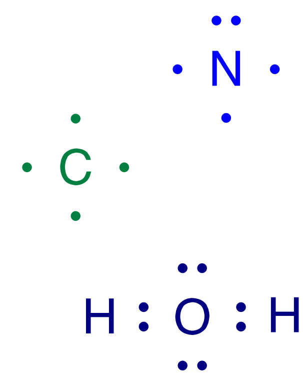
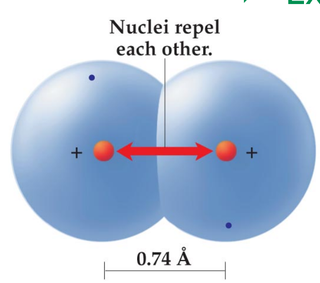
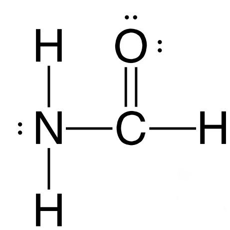
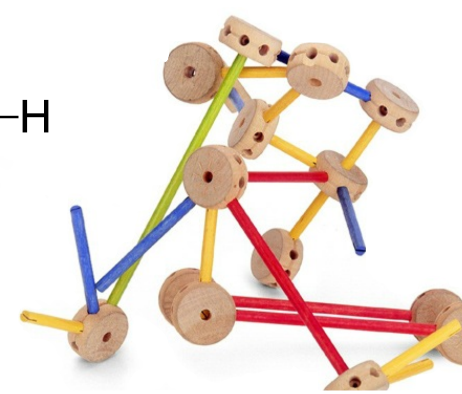




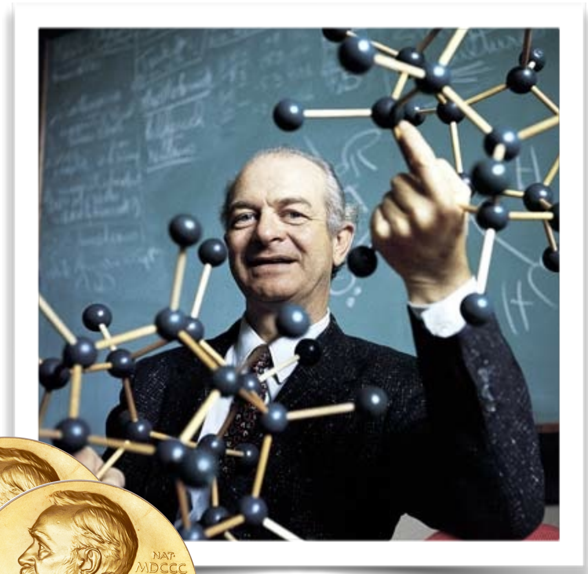


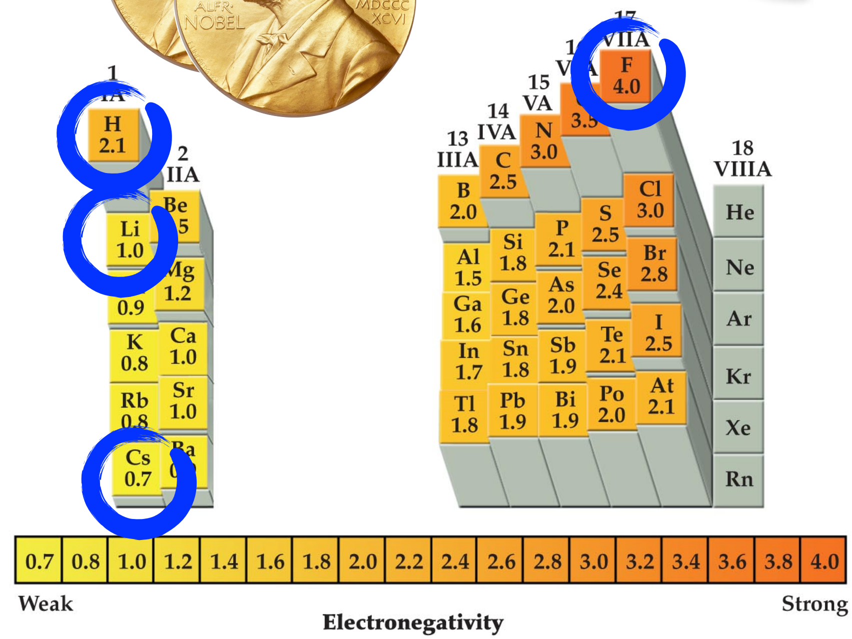




The Pauling Electronegativity Scale

- Electronegativity is a property of atoms <u>within a molecule</u> 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 <u>memorize four electronegativity</u> 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



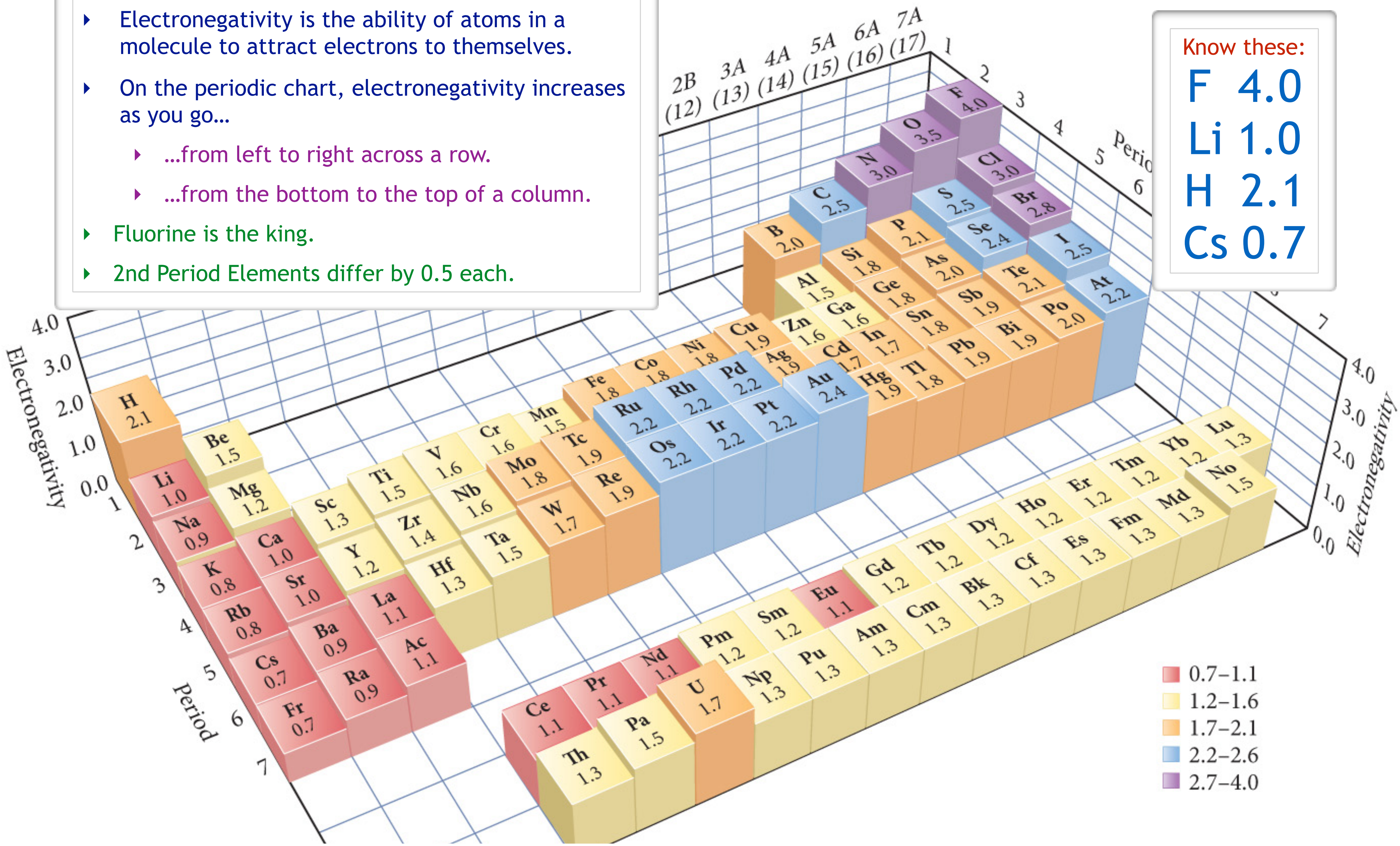


Electronegativity Trends

- 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.

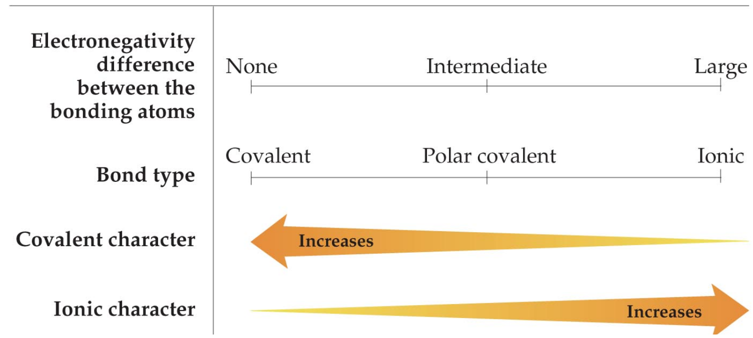
Know these:

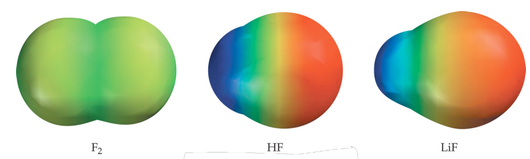
F 4.0
Li 1.0
H 2.1
Cs 0.7



Identifying Bonding Types

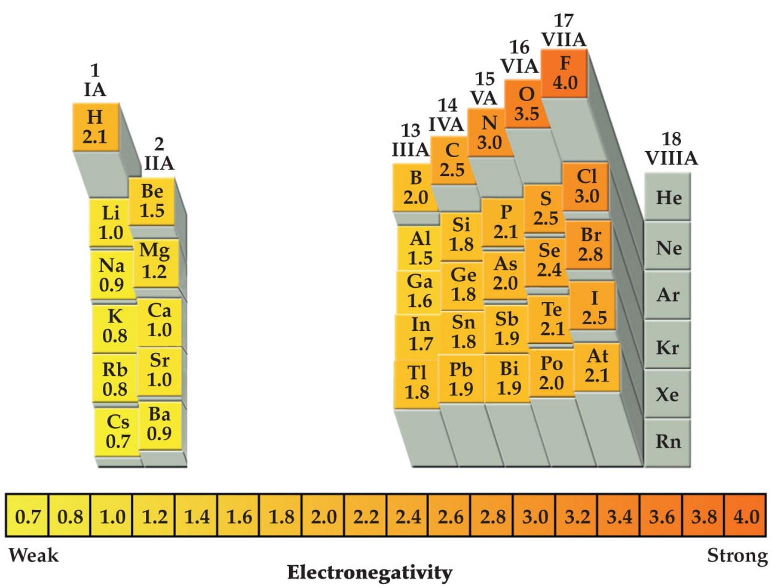
- Lewis dot structures assume all bonds are covalent bonds.
- They're not.
- Bonding indicated by Lewis structures may turn out to be either:
  - Covalent (no dipole on the bond)
  - Polar Covalent (dipole along the bond)
  - Ionic (bond snaps and atoms become charged)
- Use the difference in electronegativity (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.

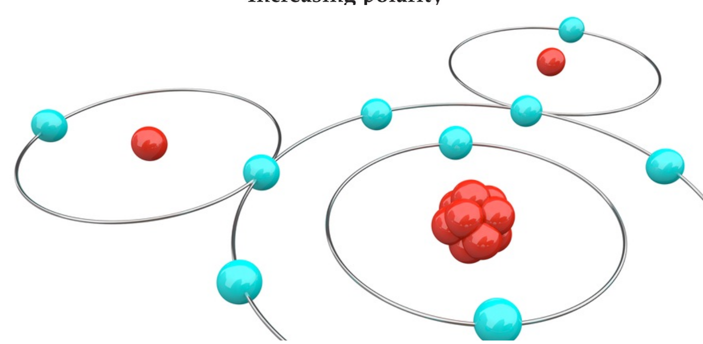




Bond	H—H	Cl—H	O—H	F—H
Electonegativity values of atoms	2.1 2.1	3.0 2.1	3.5 2.1	4.0 2.1
	2.1 −2.1	3.0 −2.1	3.5 −2.1	4.0 −2.1
ΔEN	0	0.9	1.4	1.9
Type of bond	Covalent	Polar covalent		

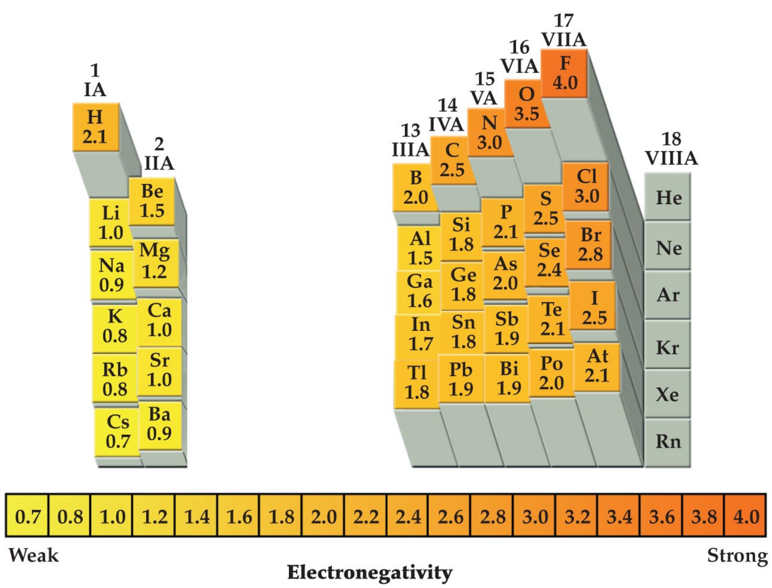
Increasing polarity





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.

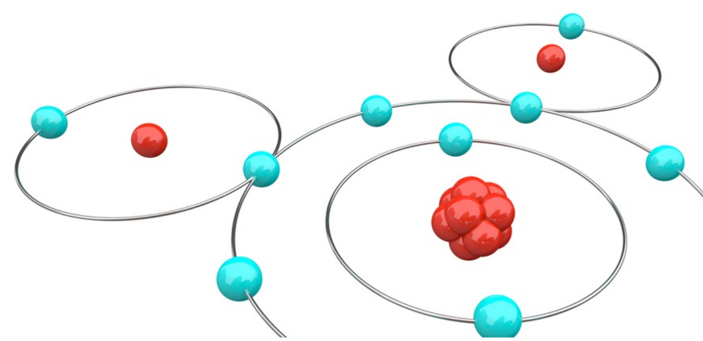


(PCl_3) P — Cl Δ EN = 0.9 Polar Covalent

(PH_5) P — H Δ EN = 0 Covalent

(Mg_3P_2) P — Mg Δ EN = 0.9 Polar Covalent

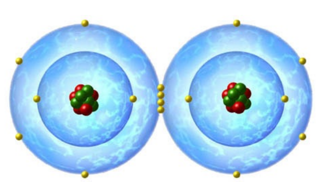
(MgO) O^{2-} Mg^{2+} Δ EN = 2.3 Ionic

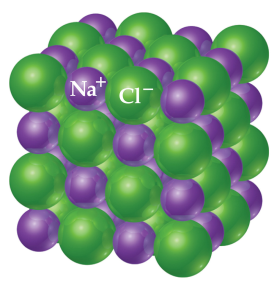


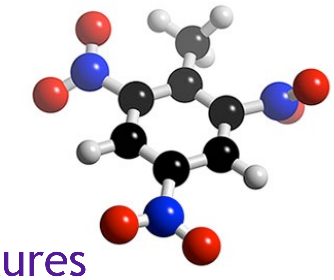
Ch12

Chemical Bonds

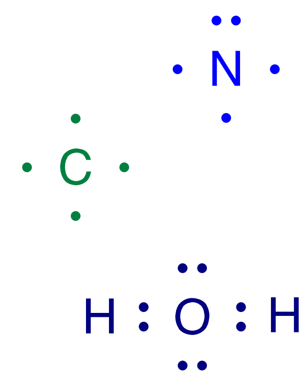
- Atoms to Molecules
  - Composition, Connectivity & Shape
  - Bonding (connectivity)
    - Metallic, Ionic & Covalent
- Lewis Symbols
  - Dots for valence Electrons
  - The octet rule
    - Cations
    - Anions
- Ionic Bonds
- Covalent Bonds
  - Bonding Pairs
    - Lone Pairs
  - Multiple Bonds

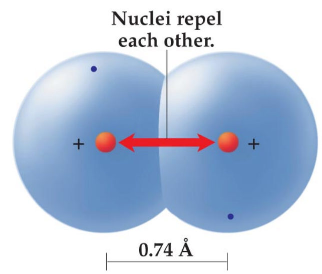


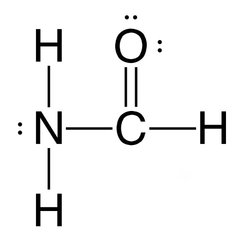


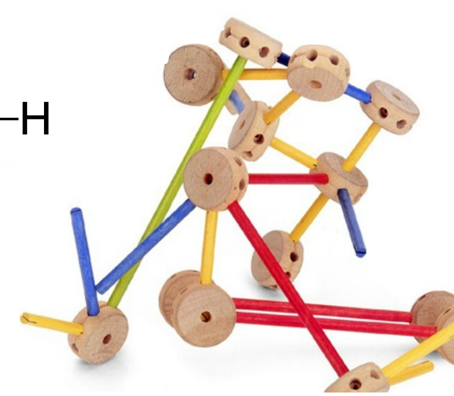


- Polar Covalent Bonds
  - Bond Dipoles
  - Electronegativity Scale
- How to Create Lewis Structures
  - Five Steps.
    - Take stock.
    - Draw a skeleton.
    - Distribute Electrons.
    - Push Electrons.
    - Evaluate Result.
  - Formal Charge
    - Resonance
    - Exceptions to the Octet Rule



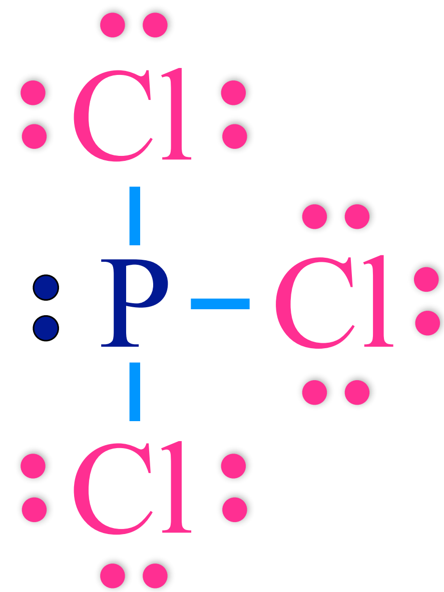




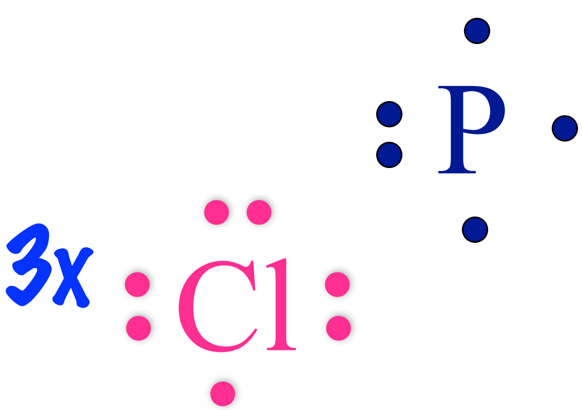


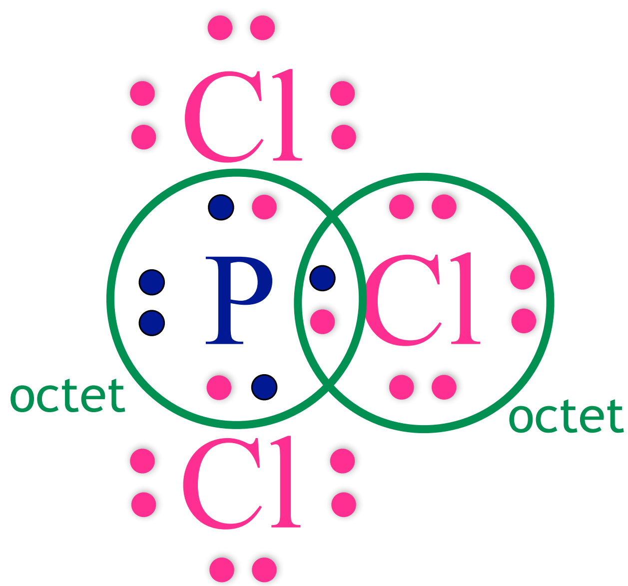
Lewis Structures

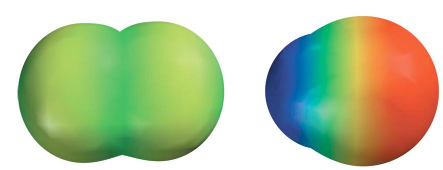
- A compound is formed by creating bonds between atoms.
- A compound is the result of atoms entangling their valence electrons, forming bonds.
- A Lewis structure is a description of a compound that shows where all the electrons of the atoms end up when the valence shells of the atoms entangle (form 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



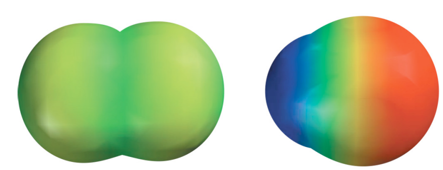




How to make a Lewis Structure:

- 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
  - Step 2: Draw a Simple Skeleton
  - Step 3: Fill in the Octets
  - Step 4: Push LP's into Bonds
    - (if needed)
  - Step 5: Show any Charge

CH_2O



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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.
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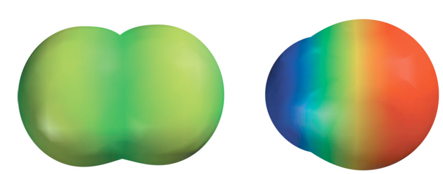
1 C	$4e^-$
2 H	$2e^-$
1 O	$6e^-$
+ No Charge	$0e^-$
	$12e^-$

CH_2O



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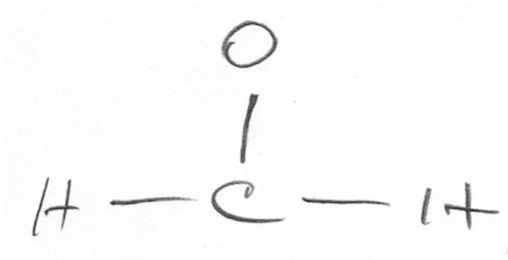
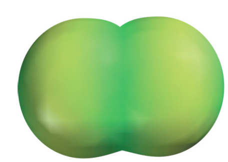
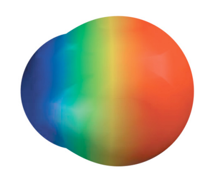
	1 C	$4e^-$
	2 H	$2e^-$
	1 O	$6e^-$
+	No Charge	$0e^-$
		$12e^-$
−	3 bonds	$6e^-$
		$6e^-$

CH_2O



2. Draw a Simple Skeleton: The central atom is the *least* electronegative element that isn't hydrogen. Connect the outer atoms to it by single bonds.





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	1 C	$4e^-$
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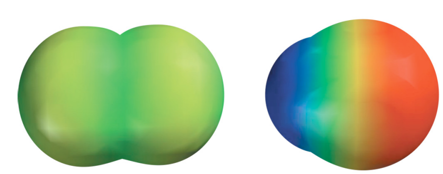
	1 O	$6e^-$
+	No Charge	$0e^-$
		$12e^-$
−	3 bonds	$6e^-$
		$6e^-$
−	3 lp's	$6e^-$
		0

CH_2O

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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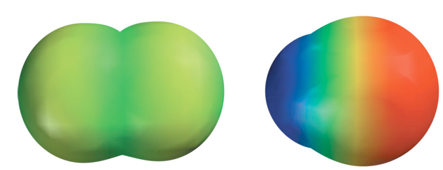
CH_2O

	1 C	4e⁻
	2 H	2e⁻
	1 O	6e⁻
+	No Charge	0e⁻
		12e⁻
−	3 bonds	6e⁻
		6e⁻
−	3 lp's	6e⁻
		0

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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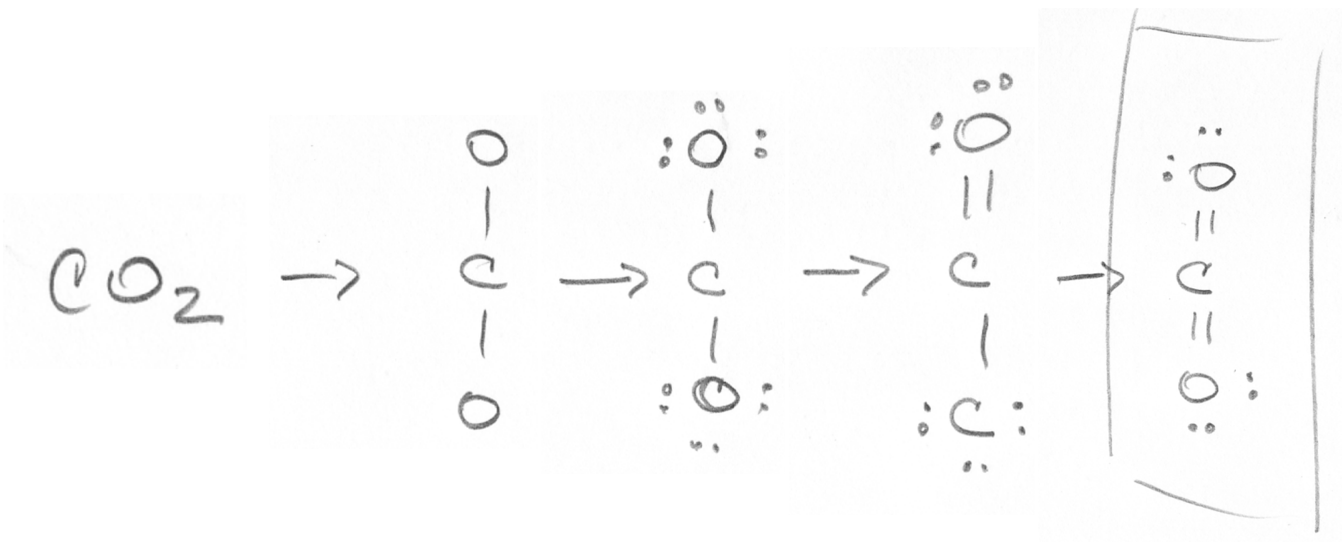
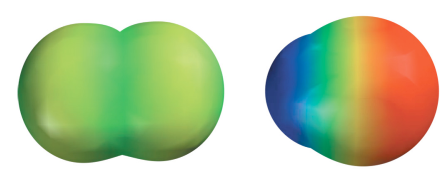
    - (if needed)
  - Step 5: Show any Charge

1 (C) $4e^-$
2 (O) $+12e^-$
$16e^-$

2 bonds $-4e^-$
$12e^-$

6 LP. $-12e^-$
$0e^-$





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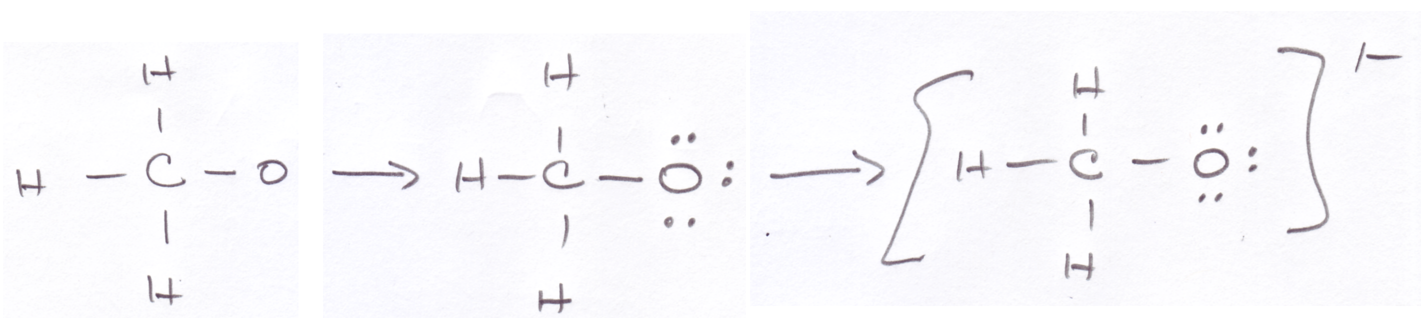
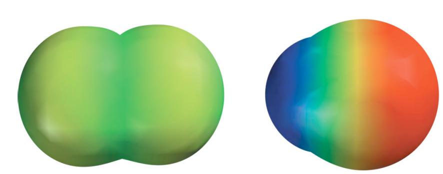
    - (if needed)
  - Step 5: Show any Charge

C	$4e^-$
3 (H)	$3e^-$
O	$6e^-$
-1 chg	$1e^-$
	$14e^-$

4 bonds	$8e^-$
	$6e^-$

CH_3O^-





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

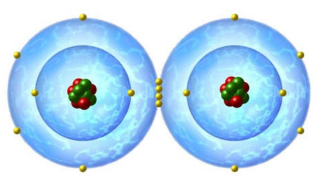
NH_4^+

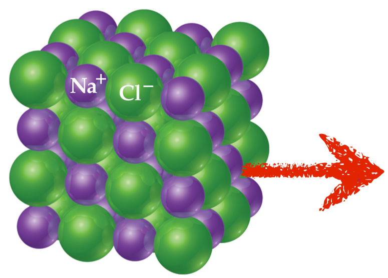
$CHOCH_3$

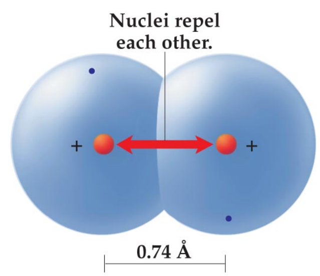
Ch12

Chemical Bonds

- Atoms to Molecules
  - Composition,
    Connectivity & Shape
  - Bonding (connectivity)
    - Metallic, Ionic & Covalent
- Lewis Symbols
  - Dots for valence Electrons
  - The octet rule
    - Cations
    - Anions
- Ionic Bonds
- Covalent Bonds
  - Bonding Pairs
    - Lone Pairs
  - Multiple Bonds







- Polar Covalent Bonds
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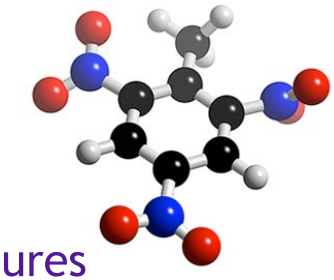
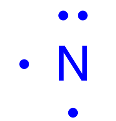
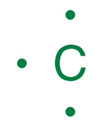
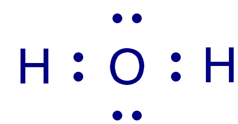
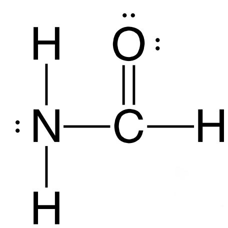
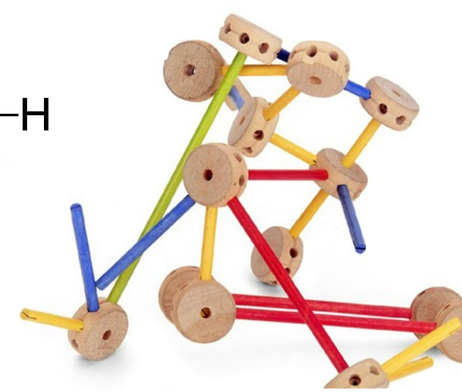








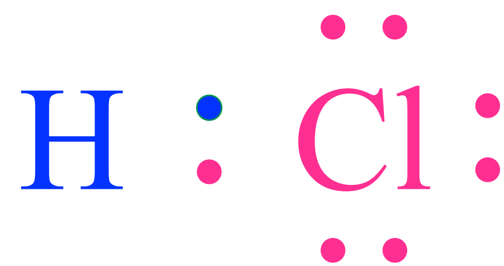




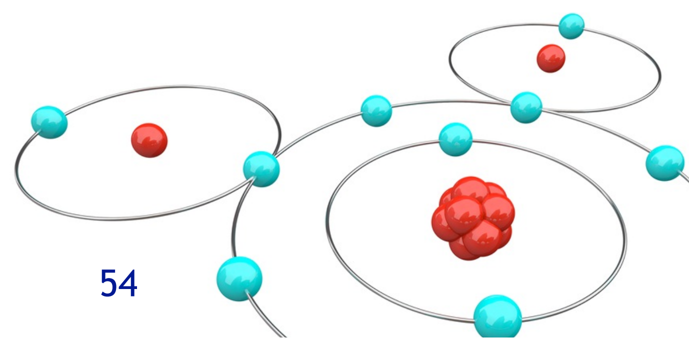
What Formal Charge is not.

- 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



Formal Charge

- Formal Charge is the formal “ownership” of electrons.
  - When we hypothesize a Lewis structure, we ask ourselves what price atom had to pay to enter into that cooperative arrangement.
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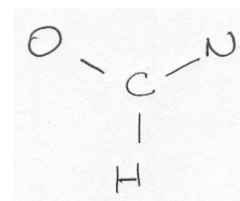
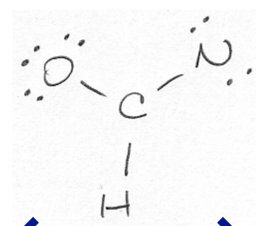
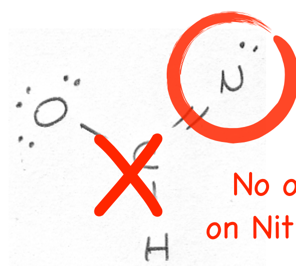
- Formal charge can be used to identify the “best” Lewis structure.
  - The best structure satisfies each atoms octet.
  - The best structure has a minimum of separation of charge.
  - The best structure places formal negative charge on the most electronegative elements.
  - The best structure places formal positive charge on the most electropositive elements.

HOCN

H 1e
O 6e
C 4e
N 5e
16e

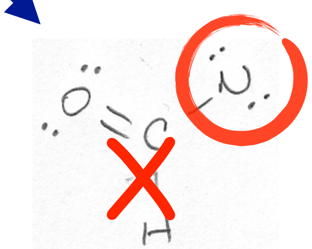






No octet
on Nitrogen!

No octet
on Nitrogen!



Neither structure is good.
Start over.

Formal Charge

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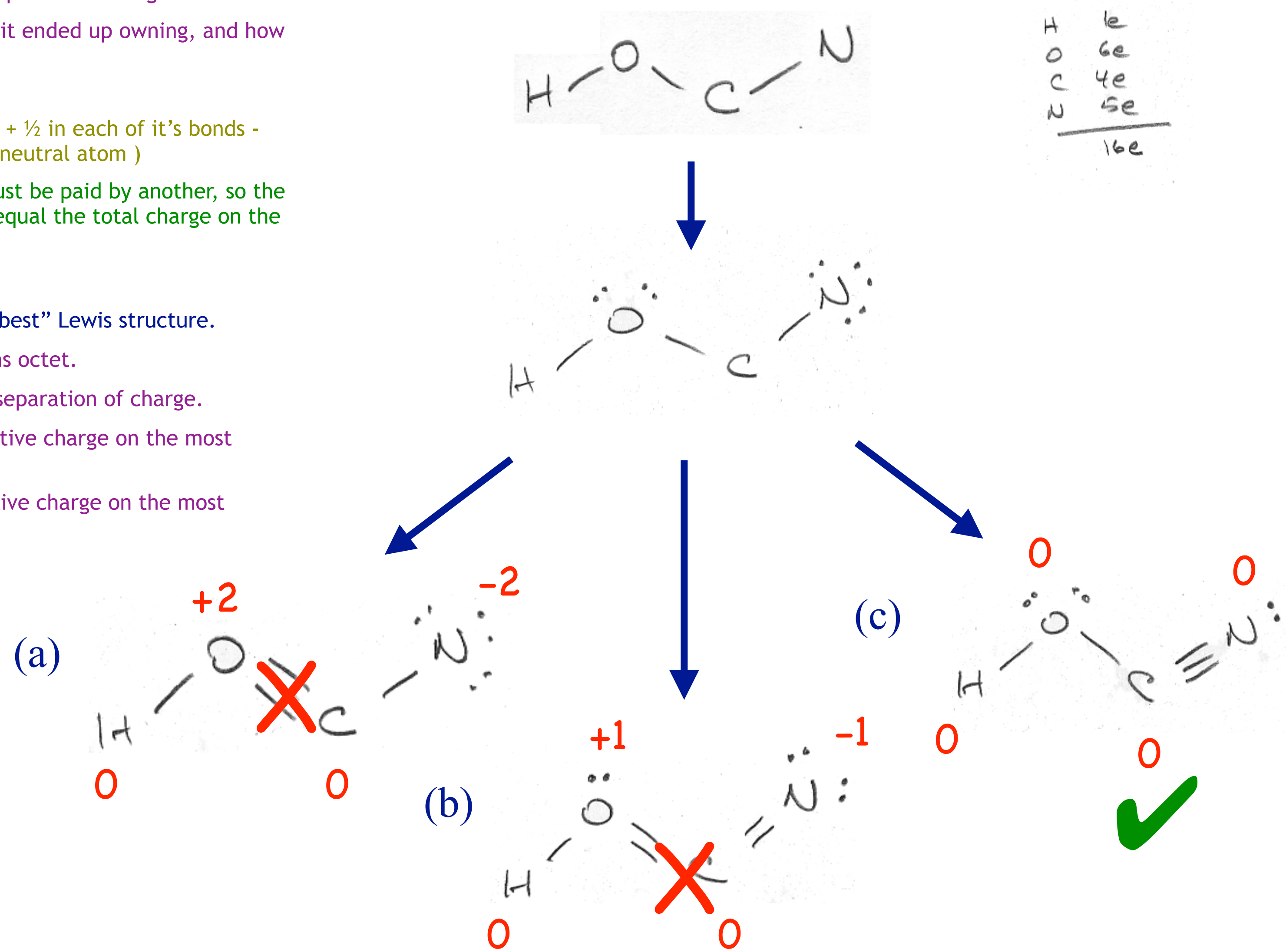
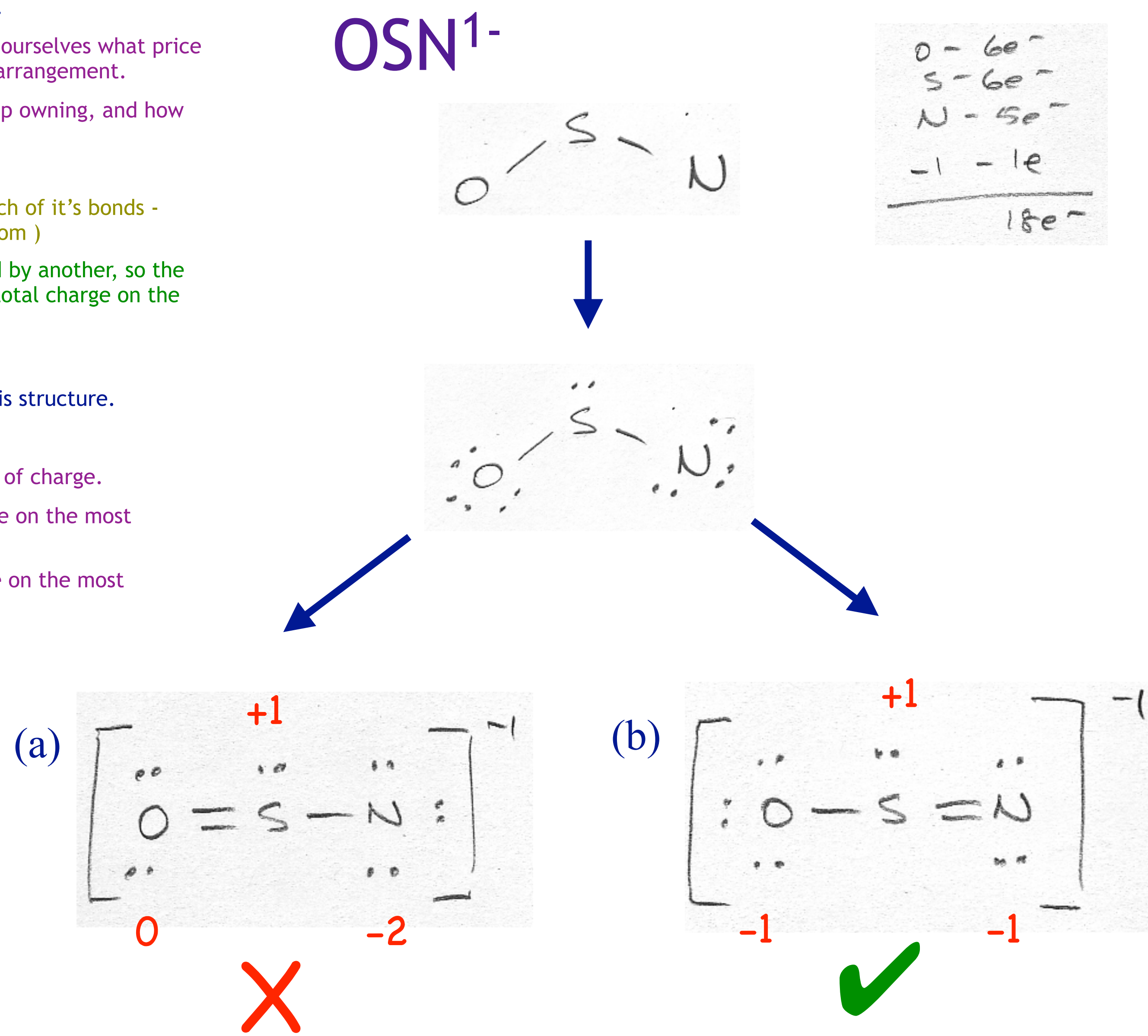
HOCN



Formal Charge

- Formal Charge is the formal "ownership" of electrons.
  - 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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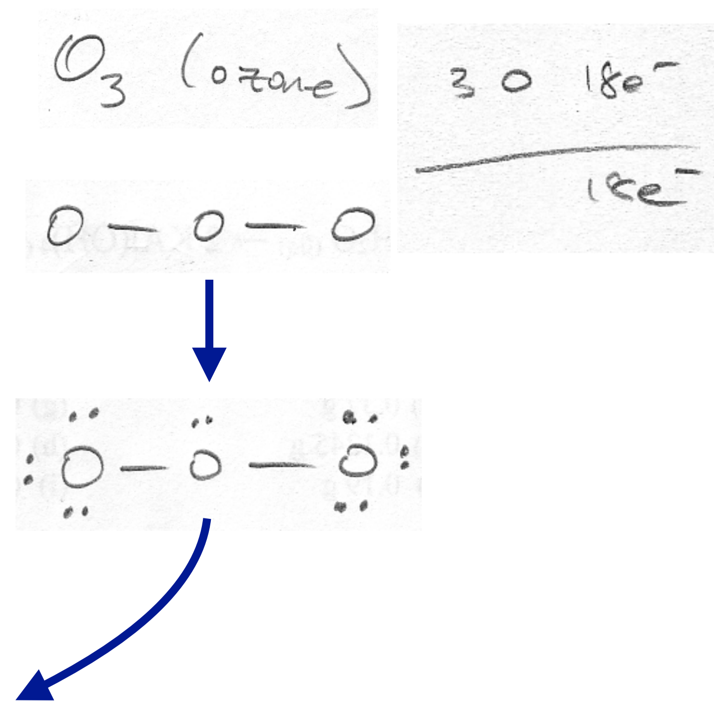

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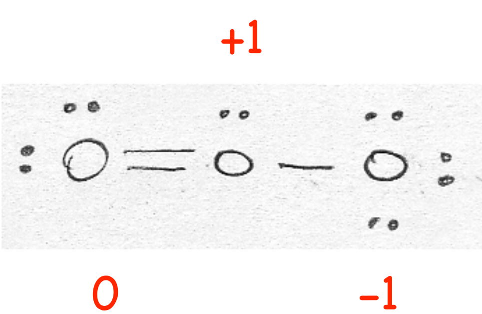

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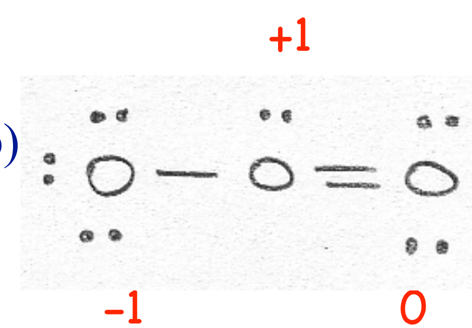

Let’s look at experiment...

Ch12

Chemical Bonds

- Atoms to Molecules
  - Composition, Connectivity & Shape
  - Bonding (connectivity)
    - Metallic, Ionic & Covalent
- Lewis Symbols
  - Dots for valence Electrons
  - The octet rule
    - Cations
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- Ionic Bonds
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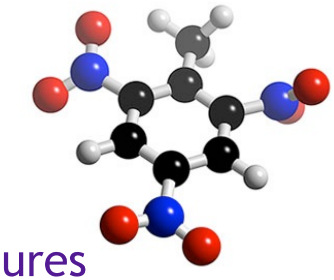

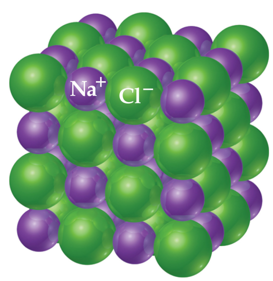

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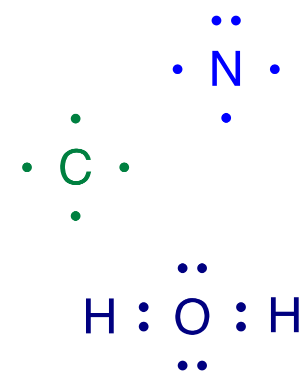

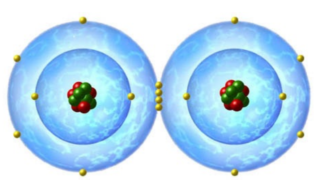

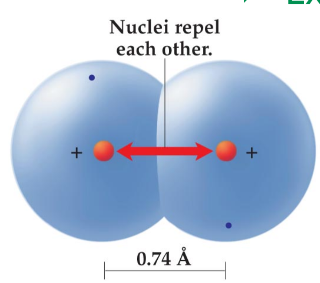

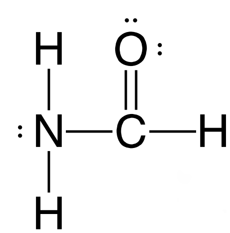

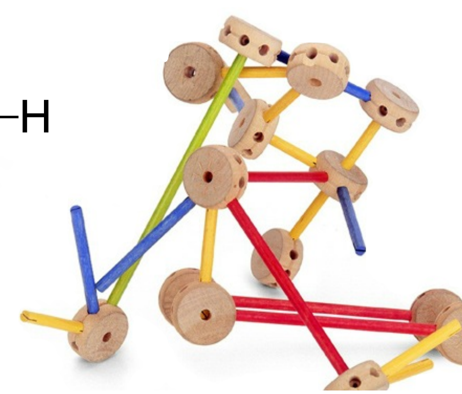

Resonance Structures

- Our Lewis analysis suggests that:
  - One of the two oxygen — oxygen bonds should be a double bond.
    - Double bonds are shorter and have more electron density between the atoms.
  - One of the terminal oxygen atoms should have greater electron density around it.
    - Three lone pairs of oxygen on one, only two on the other.
- In ozone (O_3) we find experimentally:
  - Both bond lengths are the same.
    - And the bond length is some where between what we'd expect for a double bond and single bond.
  - Electron density is evenly spread over both terminal atoms.
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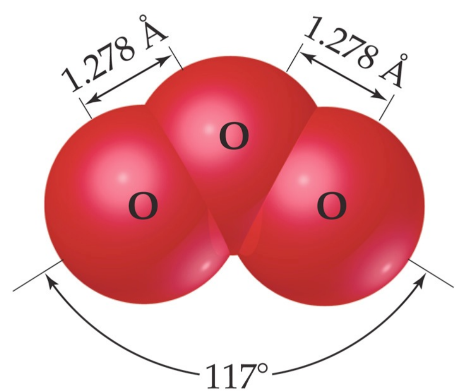

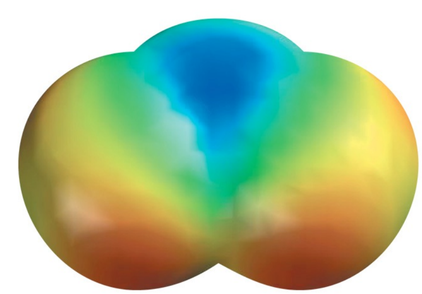

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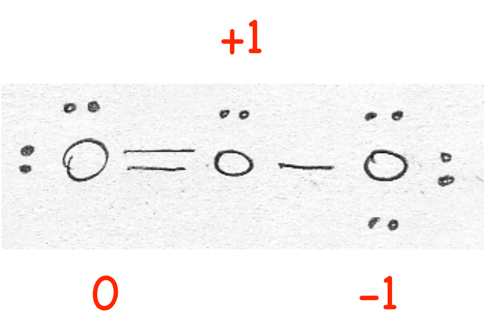

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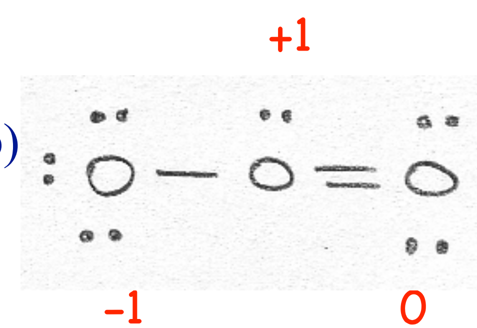

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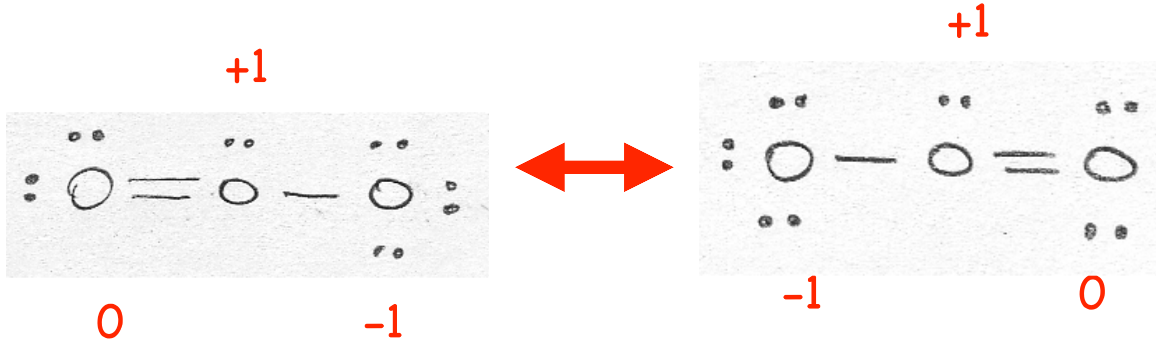

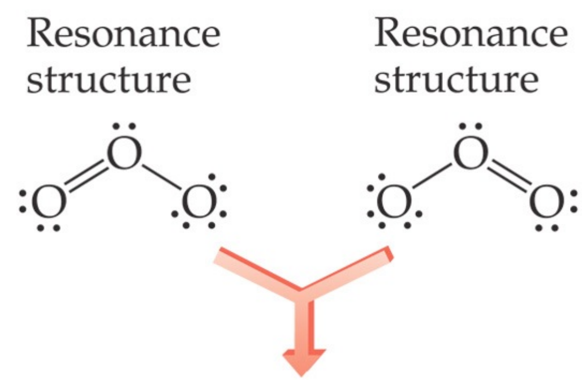

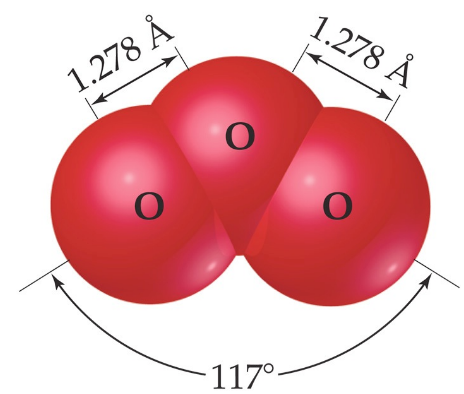

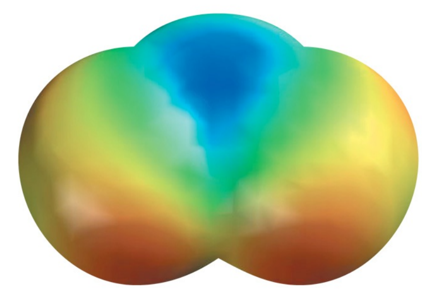

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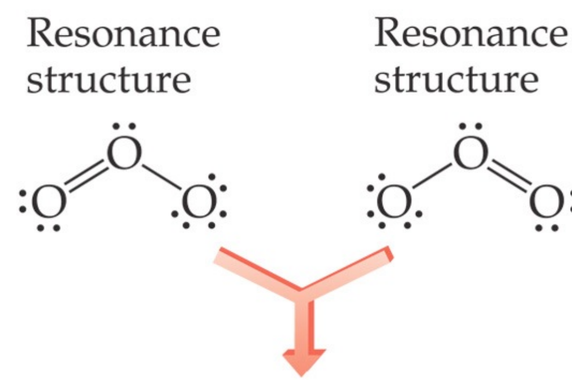
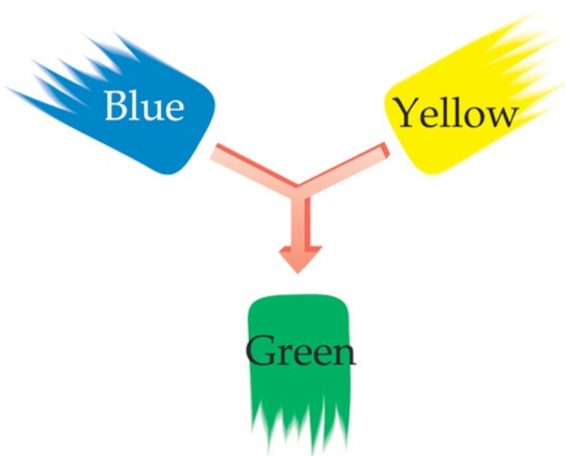
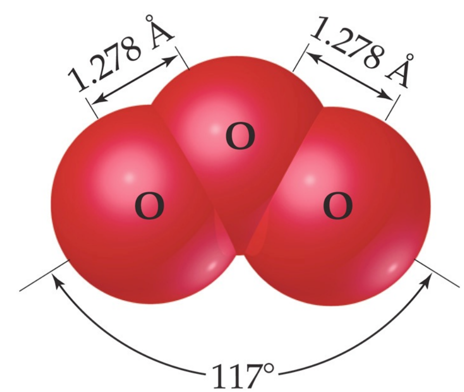
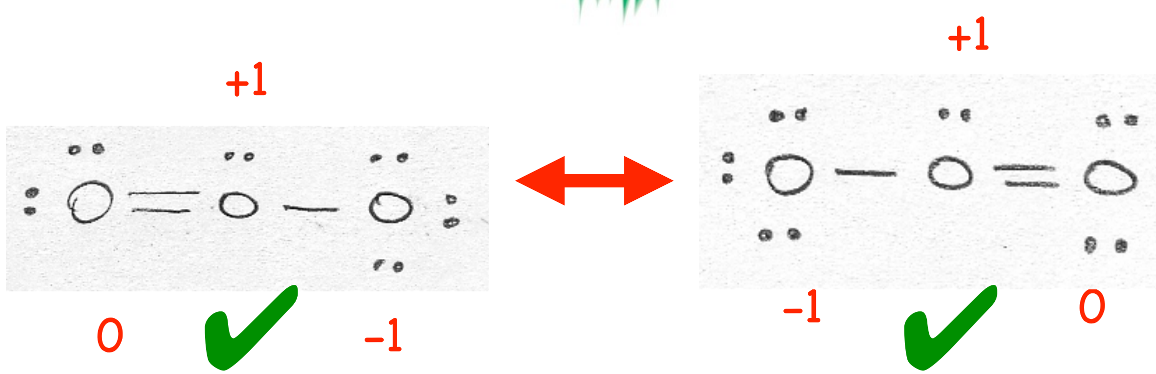
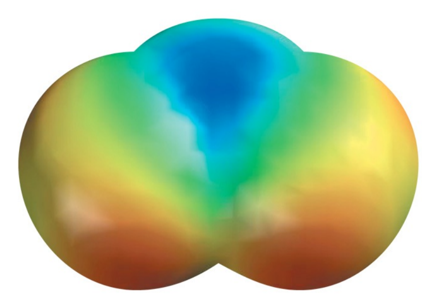
- Resonance structures are two or more structures that represent aspects of a more complex structure. We use ↔ to indicate resonance structures.
  - Note: the two structures do not interconvert. It's not like equilibrium where things are going back and forth.
  - Instead, the double headed arrow indicates that the single true structure lies between the two or more extremes.
  - The true structure is a blending of the simpler depictions.











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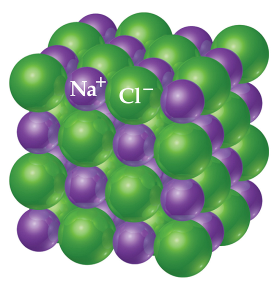

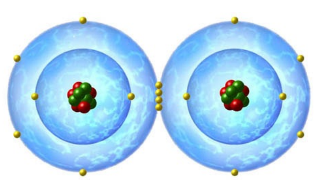

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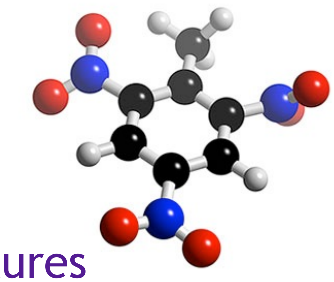
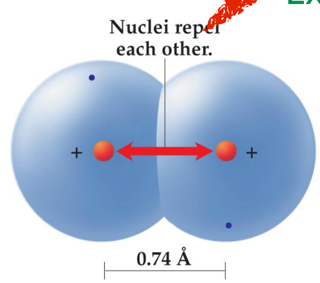
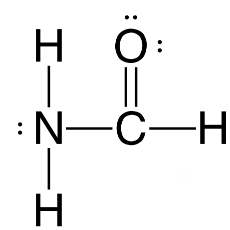


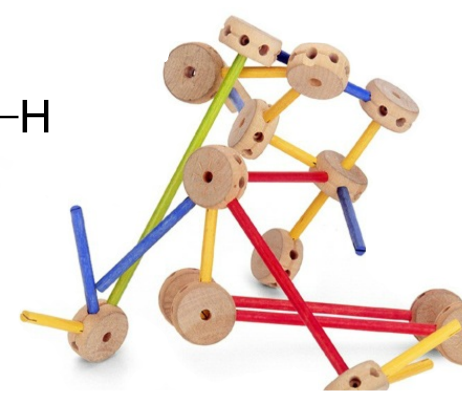
·N·

·C·

H : O : H







Octet Rule

- Atoms like a complete shell.
- Atoms will bond to share or acquire a filled valence shell.
  - for most atoms this is 8 electrons — ns^2np^6
- This produces predictable bonding tendencies:
  - atoms with 8 valence electrons form 0 bonds [Ne, Ar, Kr, etc]
  - atoms with 7 valence electrons form 1 bond [Cl, F, Br, etc]
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  - atoms with 4 valence electrons form 4 bonds [C, Si, etc]
    - 8 + 0 = 7 + 1 = 6 + 2 = 5 + 3 = 4 + 4 = **8**
  - These are tendencies, not guarantees!
- The general tendency of atoms to like a filled shell is called the octet rule.
- There are exceptions to the octet rule. Three observed exceptions are:
  1. Molecules or ions with odd numbers of electrons.
  2. Atoms that prefer less than 8 electrons.
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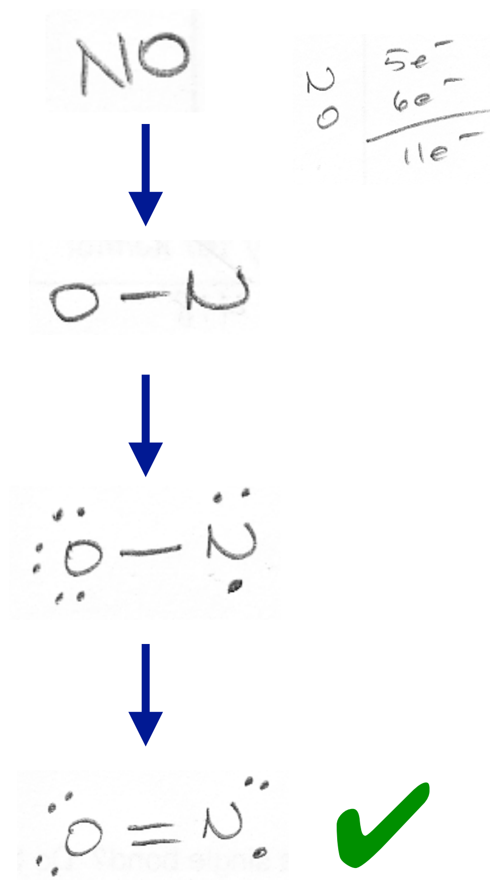

Though relatively rare and usually quite unstable and reactive, there are ions and molecules with an odd number of electrons.

Exception #2: Prefer Less than 8

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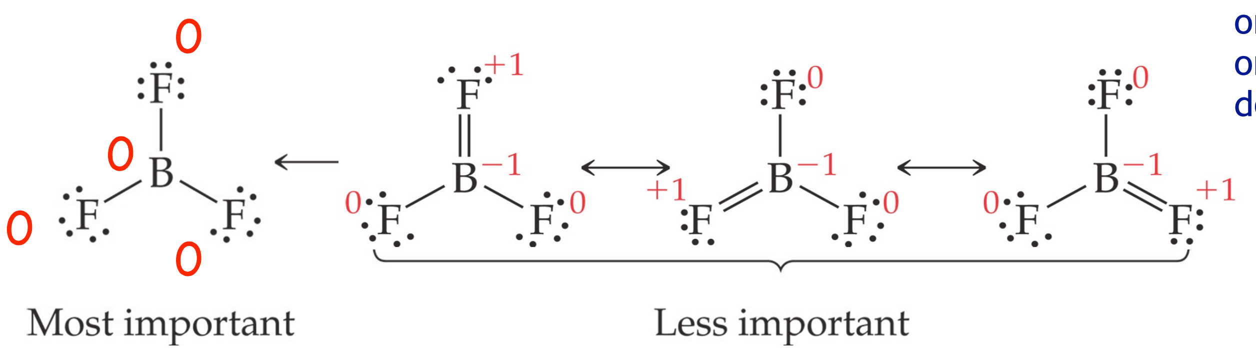

BF_3

- Consider BF_3:
  - Giving boron a filled octet places a *negative* charge on the boron and a *positive* charge on fluorine.
  - This would not be an accurate picture of the distribution of electrons in BF_3.
- Therefore, structures that put a double bond between boron and fluorine are much less important than the one that leaves boron with only 6 valence electrons.
- The lesson is: if filling the octet of the central atom results in a negative charge on the central atom and a positive charge on the more electronegative outer atom, don't fill the octet of the central atom.

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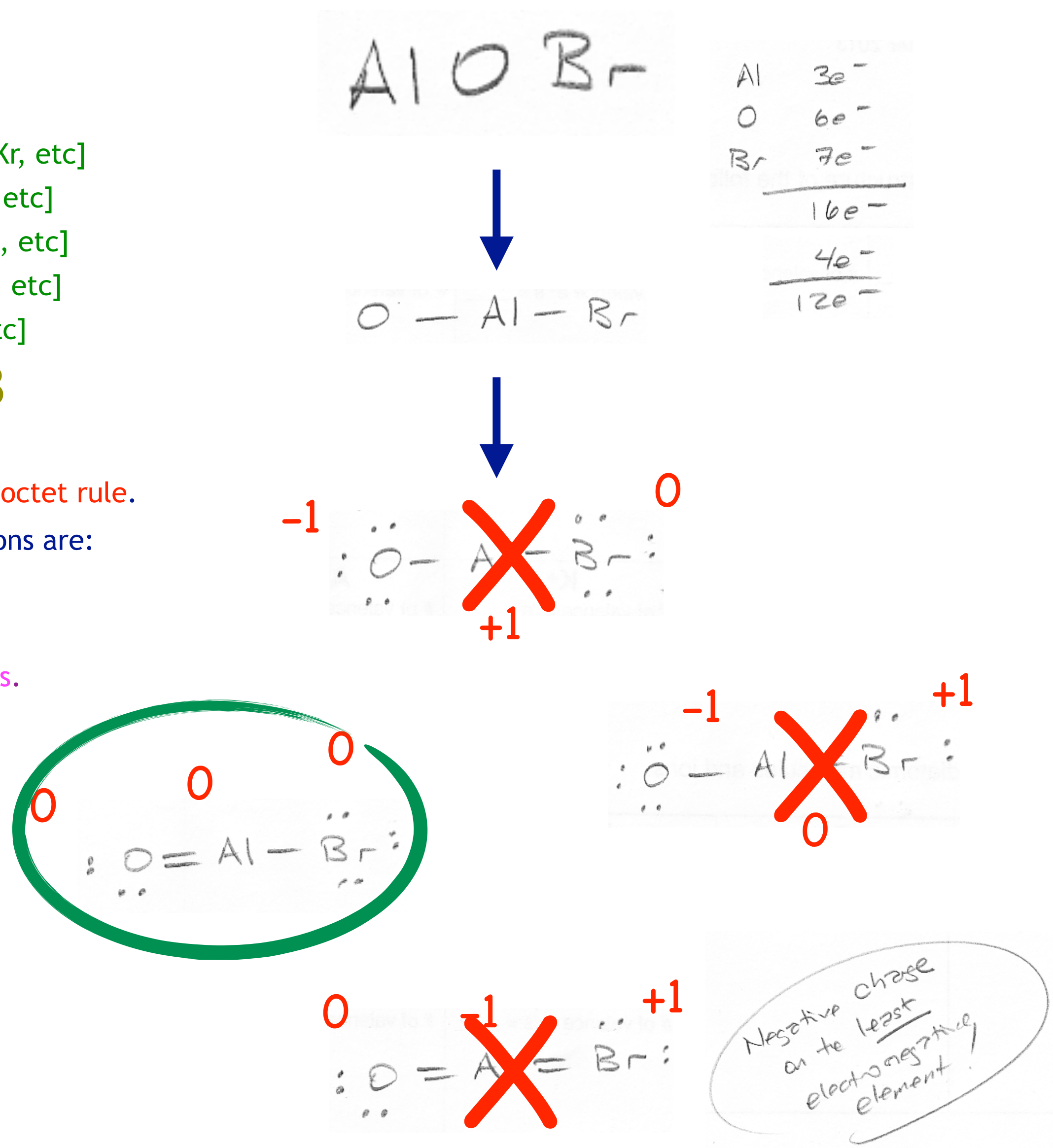

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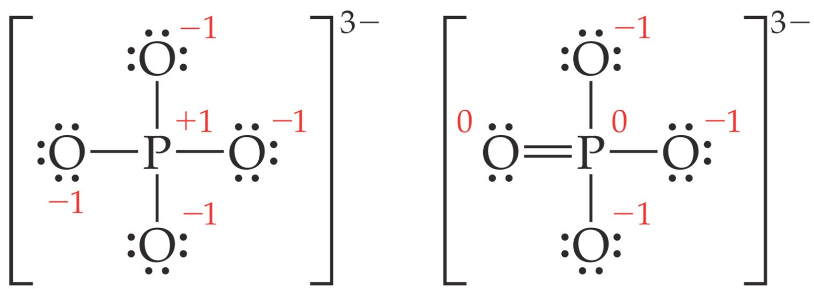
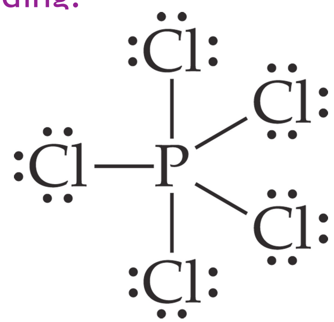


- The only way PCl5 can exist is if phosphorus has 10 electrons around it.
  - Atoms are allowed to expand the octet in the 3rd row or below.
  - Presumably d orbitals in these atoms participate in bonding.



- Even though we can draw a Lewis structure for the phosphate ion that has only 8 electrons around the central phosphorus, the better structure puts a double bond between the phosphorus and one of the oxygens.
- This eliminates the charge on the phosphorus and the charge on one of the oxygens.
- The lesson is: when the central atom in on the 3rd row or below and expanding its octet eliminates some formal charges, do so.

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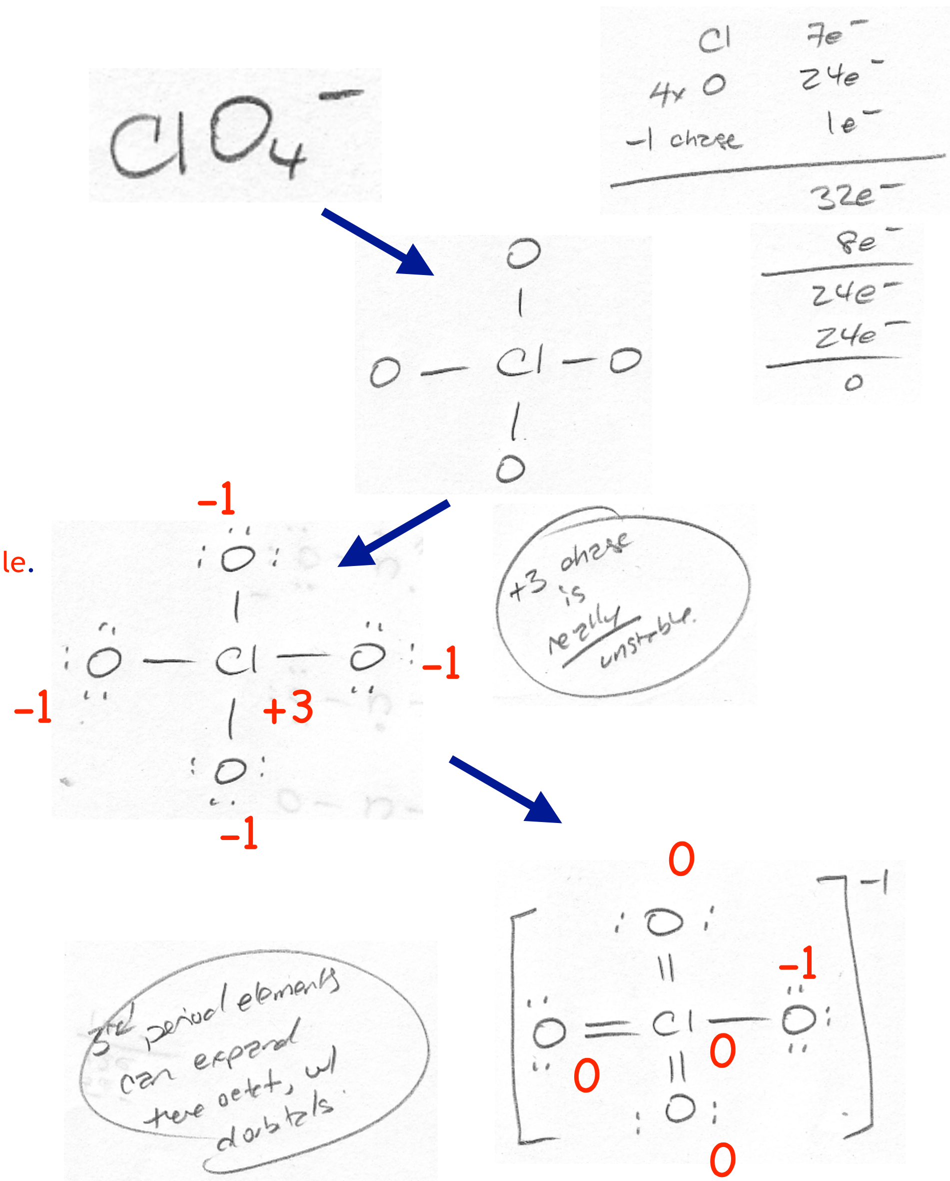

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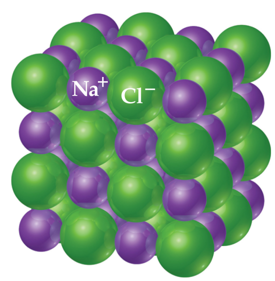

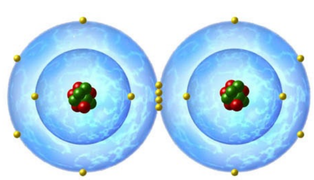

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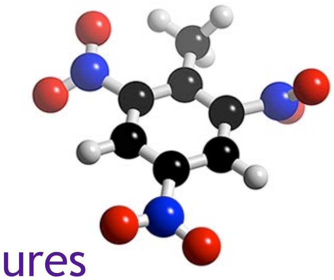

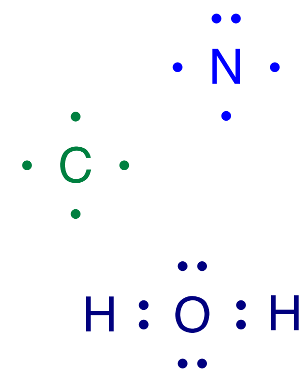

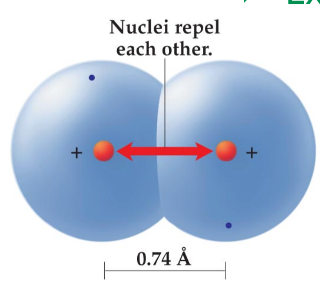

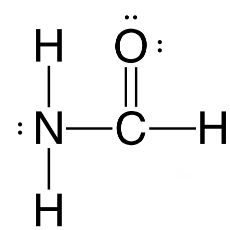

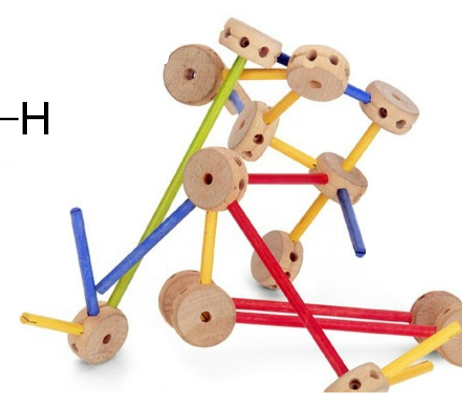

Questions?