Lewis Structures (electron dot diagrams)

Lewis Structures of Atoms

- The chemical symbol for the atom is surrounded by a number of dots corresponding to the number of valence electrons.

Number of Valence Electrons	1		2		3	4	5	6	7	8
Example	Hydrogen	Group I (Alkali metals)	Helium	Group II (alkali earth metals)	Group III	Group IV	Group V	Group VI	Group VII (Halogens)	Group VIII except Helium (Noble Gases)
Lewis Structure (electron dot diagram)	H•	Li•	He::	Be::	•B•	•C••	•N••	•O••	••F••	••Ne••

Lewis Structures for Ions of Elements

- The chemical symbol for the element is surrounded by the number of valence electrons present in the **ion**. The whole structure is then placed within square brackets, with a superscript to indicate the charge on the ion.
- Atoms will gain or lose electrons in order to achieve a stable, Noble Gas (Group VIII), electronic configuration.
- Negative ions (anions) are formed when an atom gains electrons.
- Positive ions (cations) are formed when an atom loses electrons.

Charge on Ion	1+		2+	3+	4+	4-	3-	2-	1-	
No. electrons gained or lost	1e lost		2e lost	3e lost	4e lost	4e gained	3e gained	2e gained	1e gained	
Example	H^+	Group I $^+$ (Alkali metals)	Group II $^{2+}$ (alkali earth metals)	Group III $^{3+}$	Group IV $^{4+}$	Group IV $^{4-}$	Group V $^{3-}$	Group VI $^{2-}$	Group VII $^{-}$ (Halogens)	H^- (hydride)
Lewis Structure (electron dot diagram)	[H]$^+$ OR H^+	[Li]$^+$ OR Li^+	[Be]$^{2+}$ OR Be^{2+}	[B]$^{3+}$ OR B^{3+}	[C]$^{4+}$ OR C^{4+}	[C]$^{4-}$	[N]$^{3-}$	[O]$^{2-}$	[F]$^-$	[H]$^-$

Lewis Structures for Ionic Compounds

- The overall charge on the compound must equal zero, that is, the number of electrons lost by one atom must

equal the number of electrons gained by the other atom.

- The Lewis Structure (electron dot diagram) of each ion is used to construct the Lewis Structure (electron dot diagram) for the ionic compound.

Examples

Lithium fluoride, LiF

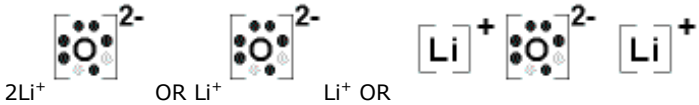
- Lithium atom loses one electron to form the cation Li^+

- Fluorine atom gains one electron to form the anion F^-
- Lithium fluoride compound can be represented as

Lithium oxide, Li_2O

- Each lithium atom loses one electron to form 2 cations Li^+ (2 electrons in total are lost)

- Oxygen atom gains two electrons to form the anion O^{2-}
- Lithium oxide compound can be represented as



Lewis Structures for Covalent Compounds

- In a covalent compound, electrons are shared between atoms to form a covalent bond in order that each atom in the compound has a share in the number of electrons required to provide a stable, Noble Gas, electronic configuration.
- Electrons in the Lewis Structure (electron dot diagram) are paired to show the bonding pair of electrons.
- Often the shared pair of electrons forming the covalent bond is circled
- Sometimes the bond itself is shown (-), these structures can be referred to as *valence structures*.

Examples

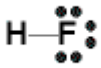
hydrogen fluoride, HF

- Hydrogen atom has 1 valence electron

- Fluorine atom has 7 valence electrons
- Hydrogen will share its electron with fluorine to form a bonding pair of electrons (covalent bond) so that the hydrogen atom has a share in 2 valence electrons (electronic configuration of helium) and fluorine has a share in 8 valence electrons (electronic configuration of neon)

- Lewis Structure (electron dot diagram) for hydrogen fluoride

OR

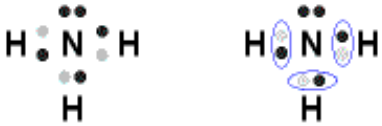


- Valence Structure for hydrogen fluoride

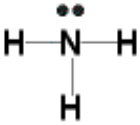
ammonia, NH_3

- Nitrogen atom has 5 valence electrons

- Hydrogen atom has 1 valence electron
- Each of the 3 hydrogen atoms will share its electron with nitrogen to form a bonding pair of electrons (covalent bond) so that each hydrogen atom has a share in 2 valence electrons (electronic configuration of helium) and the nitrogen has a share in 8 valence electrons (electron configuration of neon)
- Lewis Structure (electron dot diagram) for ammonia



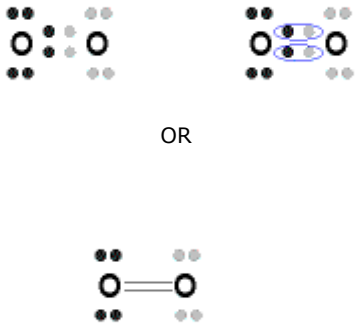
OR



- Valence Structure for ammonia

oxygen molecule, O_2

Each oxygen atom has 6 valence electrons
Each oxygen will share 2 of its valence electrons in order to form 2 bonding pairs of electrons (a double covalent bond) so that each oxygen will have a share in 8 valence electrons (electronic configuration of neon).
Lewis Structure (electron dot diagram) for the oxygen molecule



Valence structure for the oxygen molecule

describe ***ozone as a molecule able to act both as an upper atmosphere UV radiation shield and a lower atmosphere pollutant.***

- The ozone molecules in the stratosphere form a very thin layer that protects us from harmful UV radiation.

- In contrast, the ozone in the troposphere is a pollutant, even at the very low concentrations compared with the other gases. Ozone is a very reactive molecule capable of oxidising many substances.
  Fortunately most of the ozone occurs in the stratosphere.

describe ***the formation of a coordinate covalent bond.***

Revision: covalent bond

Non-metallic compounds contain covalent bonds. A covalent bond is a shared pair of electrons that keeps two atoms together. Normally one atom contributes one electron and the other joined atom contributes the other shared electron.

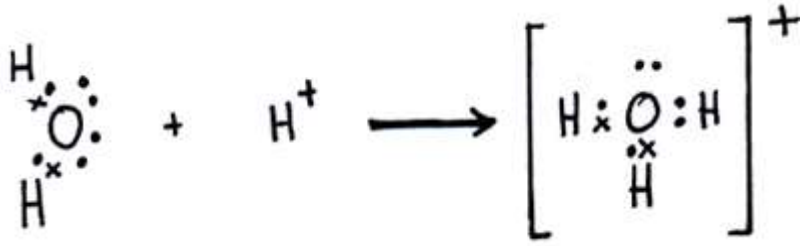
- A coordinate covalent bond forms when one atom in a species (a molecule or ion containing non-metallic atoms) provides both electrons in the covalent bond.

- Once formed this coordinate bond is indistinguishable from other covalent bonds.

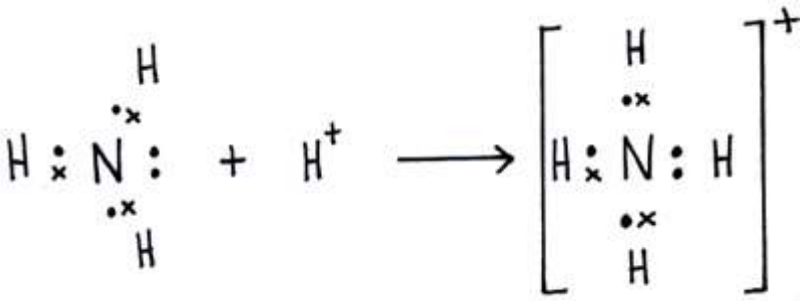
demonstrate ***the formation of coordinate covalent bonds using Lewis electron dot structures.***

- Ions, such as the hydronium H_3O^+ and the ammonium NH_4^+, contain a coordinate covalent bond. In the formation of the hydronium ion, one of the non-bonding electron pairs on the oxygen atom is used to form a covalent bond between the hydrogen ion H^+ (which has no electrons) and the oxygen atom.

  Formation of a coordinate covalent bond in the hydronium ion



  Formation of a coordinate covalent bond in the ammonium ion



compare the properties of the oxygen allotropes O_2 and O_3 and account for them on the basis of molecular structure and bonding.

Background

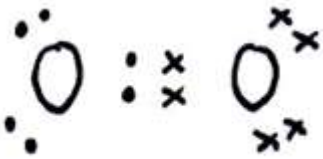
An allotrope is a different physical form of the same element, e.g. O_2 and O_3 are allotropes of oxygen.

- The chemical and physical properties differ, namely:

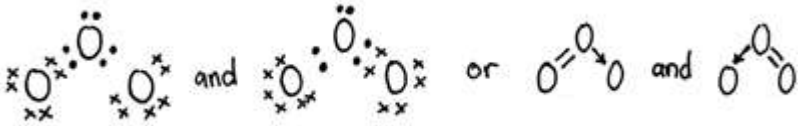
Properties	gaseous oxygen	gaseous ozone	Explanation
colour	colourless	blue	-

boiling point	–183°C	–111°C	The boiling point of diatomic oxygen is lower than that of the ozone as diatomic oxygen has a lower molecular mass requiring less energy in the boiling process.
solubility in water	sparingly soluble	more soluble than oxygen	Non-polar O_2 does not form strong intermolecular forces in the polar water. Ozone has a bent structure, which provides for some polarity of the molecule in its interaction with water.
chemical stability	far more stable than the ozone molecule	far less stable than the oxygen molecule	Ozone is easily decomposed into oxygen molecules: $2O_3(g) \rightarrow 3O_2(g)$ #More detailed information below.
oxidation ability	less powerful oxidant	more powerful oxidant	e.g. reaction with metals: oxygen forms the oxide as the only product whereas ozone reacts more readily producing the metallic oxide and an oxygen molecule.

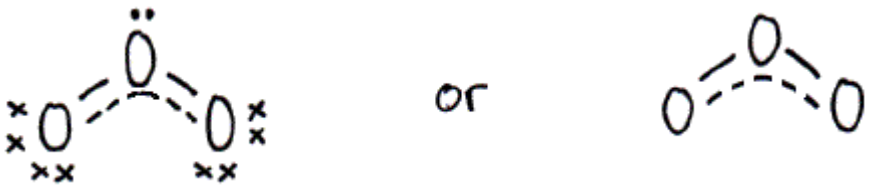
- #More detailed information regarding chemical stability:
- The oxygen molecule contains one double covalent bond O=O.
- Lewis electron dot structure for oxygen



- The ozone molecule can be represented as containing a covalent double bond and a coordinate covalent single bond. The coordinate covalent bond can be represented by an arrow.
- Lewis electron dot structure for ozone



- Measurements show that the bonds between the oxygen atoms in ozone are of equal length and strength and can be represented so:



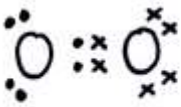
- The two identical oxygen to oxygen bonds in ozone consist of a single bond and a partial bond. This results in lower stability of the ozone molecule, compared with the diatomic oxygen molecule.

compare ***the properties of the gaseous forms of oxygen and the oxygen free radical.***

- The oxygen atom in its ground state (electrons in the lowest possible energy levels) has 3 pairs of electrons in its valence shell.

- When UV energy splits an oxygen molecule, two oxygen atom radicals are formed, i.e. they each have two electron pairs and two unpaired electrons. The energy absorbed in the splitting and the unpaired electrons make the free radical very reactive.

  Lewis electron dot structure of gaseous forms of oxygen



oxygen gas
(molecular O_2)

oxygen free
radical gas

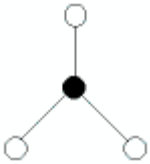
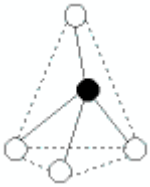
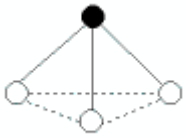
- In order of reactivity, the diatomic oxygen molecule is less reactive than the ozone molecule, which is less reactive than the oxygen free radical.

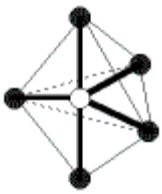
Shapes of Molecules

Key Concepts

- A molecule consists of 2 or more atoms joined by covalent bonds.
- The shape of a molecule is a description of the way the atoms in the molecule occupy space.
- A diatomic molecule, a molecule composed of only 2 atoms, must always be linear in shape as the centers of the 2 atoms will always be in a straight line.
- 'Electron Cloud' Repulsion Theory (Valence Shell Electron Pair Repulsion, VSEPR) is used to predict shapes and bond angles of simple molecules

a. an 'electron cloud' may be a single, double or triple bond, or a lone pair of electrons
b. a lone pair of electrons is a non-bonding pair of electrons
c. 'electron clouds' are negatively charged since the electrons are negatively charged, so electron clouds repel one another and try to get as far away from each other as possible
d. lone pairs of electrons exert a greater repelling effect than bonding pairs do
e. lone pair-bonding pair repulsion is greater than bonding pair-bonding pair repulsion
f. lone pair-lone pair repulsion > lone pair-bonding pair repulsion > bonding pair-bonding pair repulsion

Total Number of electron pairs	***Arrangement of electron pairs***	***Number of bonding pairs of electrons***	***Number of lone pairs of electrons***	***Shape of Molecule***	***Name of Shape***	***Bond Angle***	***Examples***
not applicable	linear	1	not applicable		linear	180°	H_2, HCl
2	linear	2	0		linear	180°	CO_2, HCN
3	trigonal planar	3	0		triganol planar	120°	BCl_3, $AlCl_3$
4	tetrahedral	4	0		tetrahedral	109.5°	CH_4, SiF_4
		3	1		trigonal pyramidal	<109.5° (bond angles in ammonia, NH_3, are 107°)	NH_3, PCl_3
		2	2		bent	<109.5° (bond angles in water, H_2O, are 105°)	H_2O, SCl_2

5	trigonal bipyramidal	5	0		trigonal bipyramidal	120° in the trigonal planar part of the molecule, 90° for the others	PCl_5
6	octahedral	6	0		octahedral	90°	SF_6

Examples

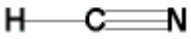
a. hydrogen chloride, HCl

HCl is composed of only 2 atoms, 1 atom of hydrogen and 1 atom of chlorine covalently bonded.
HCl is, therefore, diatomic.
All diatomic molecules are linear in shape.

H-Cl is linear in shape

b. hydrogen cyanide, HCN

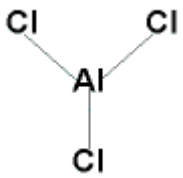
HCN is composed of 3 atoms, 1 atom of hydrogen, 1 atom of carbon and 1 atom of nitrogen covalently bonded.
Carbon, C, is the central atom in the molecule.
Carbon has 4 valence electrons (electrons that can be used in bonding).
1 of carbon's valence electrons will be used to form a covalent bond with hydrogen.
3 of carbon's valence electrons will be used to form 3 covalent bonds with nitrogen (a triple bond).
The central carbon atom therefore has no lone pairs of electrons.
The bonding pairs will repel each other as much as possible, so the molecule will be linear.



HCN is linear in shape.

c. aluminium chloride, $AlCl_3$

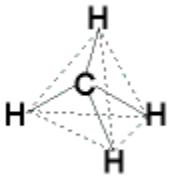
$AlCl_3$ is composed of 4 atoms, 1 atom of aluminium and 3 atoms of chlorine.
Aluminium, Al, is the central atom in the molecule.
Aluminium has 3 valence electrons (electrons that can be used in bonding).
Each of the aluminium's valence electrons will be used to form a covalent bond with each chlorine atom.
The central aluminium atom will therefore have no lone pairs of electrons and 3 bonding pairs of electrons.
The bonding pairs of electrons will repel each other as much as possible, so the molecule will be trigonal planar.



$AlCl_3$ is trigonal planar in shape.

d. methane, CH_4

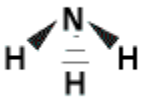
CH_4 is composed of 5 atoms, 1 atom of carbon and 4 atoms of hydrogen covalently bonded.
Carbon, C, is the central atom in the molecule.
Carbon has 4 valence electrons (electrons that can be used in bonding).
Each of carbon's 4 valence electrons will form a bonding pair with 1 of hydrogen's electrons.
The central carbon atom will therefore have no lone pairs of electrons and 4 bonding pairs of electrons,
The bonding pairs of electrons will repel each other as much as possible, so the molecule will be tetrahedral.



CH_4 is tetrahedral in shape.

e. ammonia, NH_3

NH_3 is composed of 4 atoms, 1 nitrogen atom and 3 hydrogen atoms covalently bonded.
Nitrogen, N, is the central atom in the molecule.
Nitrogen has 5 valence electrons.
3 of nitrogen's valence electrons will be used to form bonding pairs of electrons with hydrogen (3 covalent bonds).
These bonding pairs repel each other equally and will try to get as far away from each other as possible.
2 of nitrogen's valence electrons will be unused for bonding, these are a lone pair of electrons.
lone pair-lone pair repulsion is greater than bonding pair-bonding pair repulsion, so the lone pair pushes the bonding pairs closer together than in a tetrahedral arrangement of the 'electron clouds'.
This distorted tetrahedral arrangement is called trigonal pyramidal.



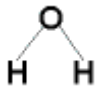
NH_3 is trigonal pyramidal in shape.

In this representation, the solid triangles represent bonds coming out of the plane of the screen, the broken lines represented a bond going behind the plane of the screen.

f. water, H_2O

Water is composed of 3 atoms, 1 atom of oxygen and 2 atoms of hydrogen covalently bonded.
Oxygen, O, is the central atom.
Oxygen has 6 valence electrons.
2 of oxygen's electrons will be used to form bonding pairs of electrons with hydrogen (2 covalent bonds).
These bonding pairs repel each other equally and will try to get as far away from each other as possible.
4 of oxygen's valence electrons will not be used for bonding, these will remain as 2 lone pairs of electrons.
These lone pairs of electrons repel each other equally and will try to get as far away from each as possible.

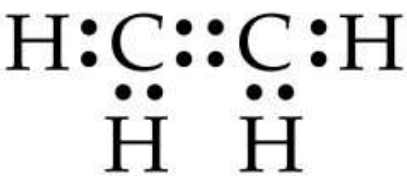
lone pair-lone pair repulsion is greater than lone pair-bonding pair or bonding pair-bonding pair repulsion, so the lone pairs of electrons push the bonding pairs of electrons closer together than in a tetrahedral arrangement of the 'electron clouds'.
This distorted tetrahedral arrangement is call bent.

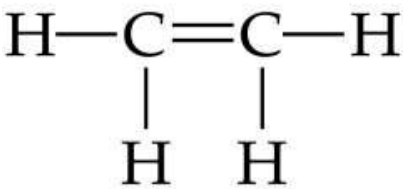


H_2O is bent in shape.

In this representation, solid lines represent bonds that are in the same plane as the screen.

Module 4 Part B: Dot Structures of Molecules Study Notes:





In Section 9.4 of the 6th edition of Kotz (CHM 2045C) there is an excellent explanation of covalent bonds and drawing dot structures of molecules. We will focus in Part B only on those molecules which can be explained by the octet rule for the nonmetals (and duet rule for hydrogen). Page 384-5 lists five steps where you do a little math in step 2 to calculate all the valence electrons and the number of bonds and lone pairs. Examples 9.2 and 9.3 show simple binary molecular compounds. Please note the Problem-Solving tip on page 388. Tables 9.4 and 9.5 show the comparison of molecules and polyatomic ions.

Kotz's five steps (#2 was expanded to Steps 2 and 3 below):

1. **Decide on the central atom (usually not oxygen or hydrogen). The central atom is usually the one with the lowest electron affinity. In formaldehyde, CH_2O, the central atom is carbon.**

2. **Determine the total number of valence electrons in the molecules or the ion. I a neutral molecule this number will be the sum of the valence electrons of each atom. For a negative ion add the charge to this total number. For a positive ion subtract the positive charge from this total number. For CH_2O: C=4, H=1(x2) , O=6 this would be 4+2+6 = 12 total valence electrons.**

3. **Take this total number of electrons and divide by two to determine the number of electron pairs. For CH_2O: 12/2 = 6 electron pairs**

4. **Place one pair of electrons between each pair of bonded atoms to form a single bond. You can either show a pair of dots, or draw a single stick between the two atoms to represent the single covalent bond.**
5. **Use any remaining pairs as lone pairs around each atom (except hydrogen) so that each atom is surrounded by eight electrons. (There is never a lone pair on a carbon except in Carbon moxide)**
6. **If the central atom has fewer than eight electrons at this point, move one or more of the lone pairs on the terminal atoms in a position intermediate between the center and the terminal atom to form multiple bonds. (As a general rule double or triple bonds are formed when both atoms are from the following nonmetals: C, N, O, S. That is, bonds such as C=C, C=n, C=O, S=O will be incountered frequently.**

In the Kotz 7th edition Chapter 9 has become Chapter 8 as the two atomic theory chapters 7& 8 have been combined into one chapter 7. The five steps are on pages 353-4 and example 8.1 should be studies on pages 354-355.

McMurray's Text (CHM 2045C) has Covalent Bonds and Molecular structure in Chapter 7. In section 7.5 McMurray summaries the dot structures of compounds of the nonmetals in the second row of the periodic table pages 229-232. The mathematical process similar to Kotz's six steps above is found on pages 235-236.

Brady's text (CHM 2045C) covers covalent bonding in Chapter 9: Chemical Bonding-General Concepts. Brady covers drawing dot/stick structures of molecules in section 9.7 On page 377, the six step similar to the above are listed.

In the CHM 1020 text, Hill, (***Chemistry for Changing Times***-11th edition) Chapter 5 discusses chemical bonds. **Covalent bonds are introduced in section 5.7. However, section 5.11(Rules for Writing Lewis Formulas) on pages 132 and 133 list the five general rules for drawing Lewis Dot Structures. Table 5.5 on page 135 is a good summary:**

TABLE 5.5 Number of Bonds Formed by Selected Elements

Electron-Dot Symbol	Bond Picture	Number of Bonds	Representative Molecules	Ball-and-Stick Models
H·	H—	1	H—H H—Cl	HCl
He:		0	He	He
·Ċ·	—C—	4	H—C(H)(H)—H H—C(=O)—F	CH_4
·N̈·	—N—	3	H—N(H)—H H—C(=N—O—H)—H	NH_3
·Ö:	—O	2	H—O—H H—C(=O)—H	H_2O
·F̈:	—F	1	H—F F—F	F_2
·C̈l:	—Cl	1	Cl—Cl H—C(H)(H)—Cl	CH_3Cl

If you still have your Corwin CHM 1025C text, (Introductory Chemistry-Concepts & Connections – 5th Edition) sections 12.4 and 12.5 beginning on page 330 has a simpler discussion. On the bootm of page 334 Corwin has the four rules similar to above

John Taylor's Method for Drawing Dot Structures

On my web site I have a length study guide for Polyatomic ions:
http://www.hccfl.edu/faculty/john_taylor/chm1025/polyions/polyionstudyguide.html

From that study guide I have the following seven steps which I reviewed the first day of class:

Using your envelope of paper atoms, assemble a reasonable dot structure of each polyatomic ion of molecular acids (not in water) using the following criteria (You may print out the following pages and cut out the atoms: **O, H, S** and **C, Cl, P, N**):

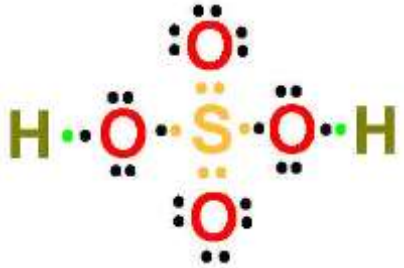
A. Place the nonmetal which is not oxygen or hydrogen in the middle of your desk.

B. **First using all single bonds, hook all oxygens in the formula to the central nonmetal** (Simple covalent or coordinate covalent bonds). **Never hook oxygen to oxygen except in peroxides**.

C. **If oxygen is present, hook the hydrogen written first in the chemical formula to an oxygen. Hydrogen requires only two electrons to fill it's orbital.** Notice the change in the polyion's charge when a hydrogen is placed on the oxygen. If hydrogen is written second in the formula after another nonmetal, then hook that hydrogen to that nonmetal, not to oxygen such as (CH_3-COOH written organically) **acetic acid** $\mathbf{HC_2H_3O_2}$ or **oxalic acid** $H_2C_2O_4$ both hydrogens are attached to the oxygens.

D. **If using all single bonds connecting the oxygen to the central nonmetal, the count of electrons around each element should total eight electrons (octet rule). This includes the element's original outer surface (valence) electrons plus the electrons being shared from the bonded element.**

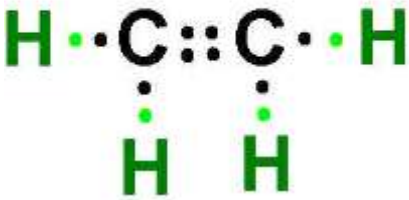
Hydrogen Sulfate (l)
Sulfuric Acid (aq)



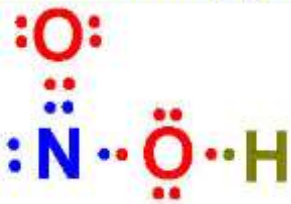
Try the following:
1. phosphate (no Plug in needed) ToolBook Demo of Phosphorus ions and molecules (Neuron plug in needed)
2. sulfate(no plug in needed) Demo of sulfur ions and molecules (Neuron plug in Needed)
3. chlorate, chlorite, hypochlorite, and perchlorate

E. If the count is 7-7, then add a second bond, a double covalent bond (four electrons being shared between two atoms.

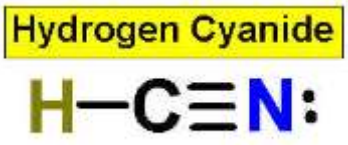
Ethene



Hydrogen Nitrite (m)
Nitrous Acid (aq)

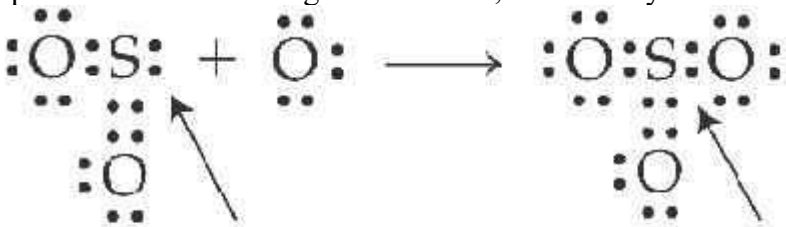


F. **If the count is 6-6, then make a triple covalent bond between the two elements (six electrons shared between the two atoms).**



G. Try the following:
1. carbonate(no Plug in)
   ToolBook Demo carbonate and molecules (Neuron Plug in Needed).
2. Nitrate
3. cyanide CN^{1-}
4. carbon dioxide CO_2
5. Nitrogen gas N_2
6. oxygen gas O_2 and ozone O_3
7. ethylene C_2H_4
8. acetylene C_2H_2

H. If the count is 8-6, then make a coordinate covalent bond. Hook the six (vacant) orbital onto an unshared pair of the eight. A coordinate covalent bond is still a single bond. In making double, triple bonds you may also use one or two coordinate covalent bonds to predict a structure using the octet rule, if necessary as in carbon monoxide.



nonbonding electron pair *coordinate covalent bond*

Table 9.4 from Kotz displays Common Hydrogen containing Compounds and Ions:

Table 9.4 Common Hydrogen-Containing Compounds and Ions of the Second-Period Elements

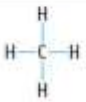
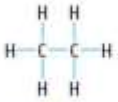
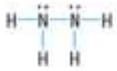
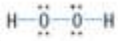
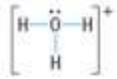
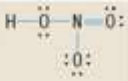
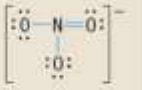
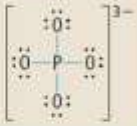
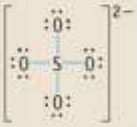
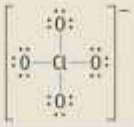
Group 4A		Group 5A		Group 6A		Group 7A	
CH_4 methane		NH_3 ammonia		H_2O water		HF hydrogen fluoride	
C_2H_6 ethane		N_2H_4 hydrazine		H_2O_2 hydrogen peroxide			
C_2H_4 ethylene		NH_4^+ ammonium ion		H_3O^+ hydronium ion			
C_2H_2 acetylene		NH_2^- amide ion		OH^- hydroxide ion			

Table 9.5 from Kotz displays common oxoacids and their anions:

Table 9.5 Lewis Structures of Common Oxoacids and Their Anions

HNO_3 nitric acid		H_3PO_4 phosphoric acid		H_2SO_4 sulfuric acid	
NO_3^- nitrate ion		PO_4^{3-} phosphate ion		HSO_4^- hydrogen sulfate ion	
$HClO_4$ perchloric acid		HOCl hypochlorous acid		SO_4^{2-} sulfate ion	
ClO_4^- perchlorate ion		OCl^- hypochlorite ion			