Lewis Dot Structures

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A **Lewis dot symbol** is a symbol in which the VALENCE electrons of an atom or simple ion are represented by dots placed around the chemical symbol of the element. Each dot represents one electron. For a single atom, we imagine an invisible box around the element symbol; each side of the box can hold a pair of electrons. Although the location of the dots is arbitrary, no side will have two dots before all sides have at least one dot.

Hydrogen	1 valence electron, 1 dot
Oxygen	6 valence electrons, 6 dots
Chlorine	7 valence electrons, 7 dots
Chloride ion	8 valence electrons, 8 dots

We will use Lewis structures to describe the chemical bonding in covalent compounds.

A COVALENT bond is a chemical bond formed by the SHARING of a pair of electrons between two atoms.

The Lewis dot structure of a covalent compound or polyatomic ion (________________________ ____) shows how the valence electrons are arranged. It is basically an accounting method that shows the connectivity of the atoms. For example, the Lewis structure for methane (CH_4) is:

Instead of using two dots to indicate the two electrons that make up the covalent bond, a DASH is substituted for the two dots that represent the two electrons.

Below is the Lewis dot structure for water, H_2O. Two hydrogen atoms (H) are separately covalently bonded to the central oxygen (O) atom. The BONDING electrons are indicated by a dash between the O and each H. The other two pairs of electrons located on O are called NON-BONDING (a.k.a. lone pair) electrons; Although they are not involved in bonding, they are extremely important and <u>must</u> be written in the Lewis structure.

SO HOW DO WE DRAW LEWIS DOT STRUCTURES?

1. The first step is to determine the total number of valence in your molecule (or ion). This is done by adding up the number of valence electrons from each of the atoms in the molecule.

> If you have an ion:
> ★ ________________________ for each _____________ charge.
> ★ __________________ electron for each _______________ charge.

2. Connect the atoms in the molecule with single bonds. Molecules tend to be symmetrical if possible.

> Also, ____________ are always _______________, ______________ are usually ______________, and _______________ tend to be in the _____________.

3. Complete the valence shell of all the atoms in the molecule. Remember, all atoms want to resemble Noble gases ("have an octet"). Each dash counts as 2 electrons. Since each pair of bonded electrons is SHARED, when assessing each atom's valence shell, we assign the dash to each atom it's bonded (i.e. we "count" each bond twice).

> Boron is an exception…it only wants _________________.
> Hydrogen only wants _________ electrons.

4. Count electrons in your structure to see if they match the available valence electrons counted in step 1. Each dash counts as 2 electrons. In this counting process, we only count each bond ONCE, since we are checking a TOTAL number of electrons, and not each atom's octet.

- If the number of valence electrons from step 1 and the number of electrons in your structure match, you have drawn an acceptable Lewis structure.

- If you have used too many electrons, your next task is to <u>remove (any) 1 lone pair from each of (any) 2 adjacent atoms and replace these 4 electrons (2 pairs = 4 electrons) with a double bond</u>. This lowers the number of electrons by 2. Make sure the atoms you choose can accommodate double bonds (i.e. H can't!)

5. Double check to make sure that 1) you have used the ______________________________ __________________, that 2) each atom ___________________, and that 3) no atom that cannot *expand its octet*, does not (i.e. ____).

6. ONCE YOU HAVE A VALID STRUCTURE, you still need to check for the **best** structure. The best Lewis structure is: ___________________________________.

   a. You must first check to see if your structure requires RESONANCE STRUCTURES.

   b. Regardless of the charge on the overall molecule/ion, you must check to see that the FORMAL CHARGES on each atom add up to the charge on the entire molecule.

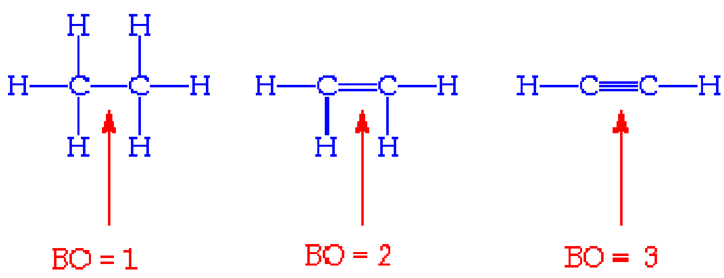
   c. Now you are ready to analyze the <u>molecular geometry</u> (VSEPR) and <u>polarity</u>.

<u>Simple examples</u>: N_2, NH_2^-, BCl_3, NH_4^+, CF_4, NH_3, H_3O^+, O_2, Cl_2, CO. Try these on your own…answers are posted.

Note For ions, you must enclose your structure in brackets, [ ] and place the charge at the top right, e.g. $[\ ]^+$. Formal charge will be added after we learn how to calculate it.

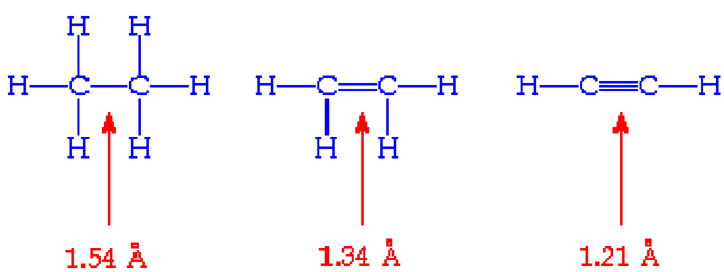
Bond Order and Bond Length

The **bond order** (BO) is equal to the ____.



The **bond length** is the ______________________________________. The greater the number of electrons between two atoms, the closer the atoms can be brought towards one another, and the shorter the bond.

The BO is an indication of the bond length WHEN COMPARING SIMILAR BOND TYPES: ____. This is an example where three different types of carbon-carbon bond lengths get shorter as the bond order gets larger:



Resonance Structures

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Sometimes, a single Lewis structure does not adequately represent the true structure of a molecule.

Consider the carbonate ion, CO_3^{2-}, which has 24 valence electrons.

Carbon is the central atom, the three oxygen atoms are bound to it and electrons are added to fulfill the octets of all the atoms.

This structure has 26 electrons but only 24 valence electrons are allowed. To remedy this we need to remove 1 lone pair from 2 adjacent atoms and replace these 2 pairs with a double bond. This will lower the number of electrons by ____ and result in the correct number of electrons. However in this case, we have 3 atoms from which to choose

Your structure would look like this if you remove lone pairs from carbon and the left-most oxygen and replace them with a double bond

or

Your structure would look like this if you remove lone pairs from carbon and the bottom oxygen and replace them with a double bond

or

Your structure would look like this if you remove lone pairs from carbon and the right-most oxygen and replace them with a double bond

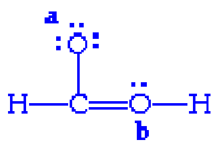
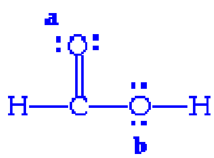
Three equivalent Lewis structures (formal charges are shown) can be drawn for the carbonate ion. The true structure of the carbonate ion is an average of the three resonance structures connected by a ______________________ and enclosed in brackets. Brackets are written _______ __________________; _______________________.

This affords a bond order for the carbon - oxygen bond of 1 ⅓ (or 1.33), which is calculated from 4 bonds, averaged over three structures.

Formal Charge

Formal charge is an accounting procedure. It allows chemists to determine the location of charge in a molecule and determine how good a Lewis structure might be. The formula for calculating formal charge (________________________) is shown below:

Consider the molecule H_2CO_2. There are two possible Lewis structures for this molecule. Each has the same number of bonds. We can determine which is better by determining which has __ __________________. It takes energy to get a separation of charge in the molecule (as indicated by the formal charge) so the structure with the least formal charge should be lower in energy and thereby be the better Lewis structure.

The <u>non-zero</u> formal charge on every atom in the molecule should be written near the atom inside a circle.

The two structures differ only in the arrangement of the valence electrons in the molecule. No atoms have been moved. These are called *resonance structures*. The better Lewis structure or resonance structure is that which has ____. HOWEVER, __________________

Try these examples on your own…answers are posted: NO_3^-, NO_2^-, SO_2, O_3

VSEPR Theory

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Valence Shell Electron Pair Repulsion Theory

VSEPR Theory is one method that chemists use to predict the shapes of molecules. This theory predicts that electron pairs, whether involved in bonds or as non-bonding pairs, will adopt a geometry (electronic shape) in which they maximize the distance from one another in order to minimize repulsions. This will result in a structure with the lowest possible energy.

Two Regions of Electron Density

When ______ regions of electron density get as far away from each other as possible, the resulting electronic shape is called ___________. The bond angle is _______°.

Three Regions of Electron Density

When ______ regions of electron density get as far away from each other as possible, the resulting **electronic shape** is called _____________. The bond angle in this arrangement is ____°.

There are two possible ***molecular shapes*** of molecules whose electronic shape is **trigonal planar**. In the first instance, all the regions are bonding regions and the shape of the molecule is the same as the electronic shape, ______________________. In the second instance, there are two bonding regions and one lone pair; the shape of molecules of this type is called ______________.

Four Regions of Electron Density

When ____________ regions of electron density get as far away from each other as possible, the resulting electronic shape is called _________________. The bond angles are __________°.

There are _________ possible ***molecular shapes*** of molecules whose electronic shape is tetrahedral. In the first instance, all the regions are bonding regions and the shape of the molecule is the same as the electronic shape, ____________________. In the second instance, there are three bonding regions and one non-bonding region, the shape of molecules of this type is called ________________. In the third instance, there are two bonding regions and two non-bonding regions; the shape of molecules of this type is called ___________.

Covalent Bonds & Molecular Polarity

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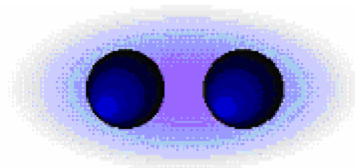
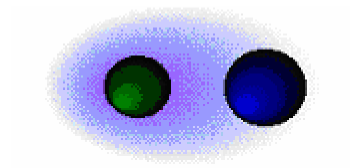
As two non-metals approach one another, the valence electrons interact and a **covalent bond** is formed between the two non-metals that ___________ a pair of electrons so that each obtains a filled valence shell.

There are two types of covalent bonds. In a _________ **covalent bond** the electrons are shared equally between the two atoms. Non-polar bonds are formed between atoms with identical ________________________.

BONDS will be non-polar if they contain ______________________________.



In a ________ **covalent bond** the electrons are shared unequally between the two atoms. In this situation, one atom has a greater ability to pull the bonding electrons towards it and is said to be more ___________________. The smaller sphere represents the more electronegative element. Recall, __________________ is the most electronegative element.



The electrons move around the nuclei with the electrons spending the majority of the time near the _______________ electronegative element. This results in a partial negative charge near the more electronegative element and a partial positive charge near the less electronegative element. This is called a _____________________.

Molecular polarity is dependent on ________________ *and* the __________________. If all the regions surrounding an atom are similar in their electronegativity and the molecule is symmetrical, the molecule will be ____________ because **symmetry cancels the dipole**. If the regions are different, or the molecule is not symmetrical, then the molecule will be ___________.

As a rule, when the **electronic and molecular shapes are the same, the molecule is symmetrical** which means the molecule is ________________.

The Best Lewis Dot Structure

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When Should I Expand the Octet?

Once you have drawn a Lewis dot structure, you should always check to see if you have drawn the BEST structure. The best structure is one that ___________________________.

So how do we accomplish this? ________________________

Look for adjacent atoms that have _____________________! If the electron deficient atom (__________________________) can expand its octet, you can move an electron pair from the electron rich atom (____________________) to a ___________ ___________between the two atoms. This will change the formal charge on these two atoms. Check to see if you can do this again. No atom can expand its octet beyond ________ electrons. Once you have minimized formal charge don't forget to look for _____________________.

Let's do an example: BrO_3^-

Summary of Lewis Dot Steps.

1. Count valence electrons
2. Arrange atoms symmetrically
3. Give all atoms an octet
4. Check to see if what you have is what you need
5. Adjust accordingly
6. Make sure you have the best structure possible
7. Assess molecular geometry, bond order, bond angles, and polarity by VSEPR theory
8. Don't forget to determine formal charges for each atom and determine if resonance structures exist for the structures you came up with.