LEWIS STRUCTURES AND VSEPR

Electronegativity - the power of an atom in a compound to draw electrons to itself. In the periodic table electronegativity increases up a group and across a row from left to right. Noble gases have very little electronegativity. i.e. F is the most electronegative atom and Cs has a very low eletronegativity.

Basic Rules

Step 1: Determine the total number of valence electrons in the molecule or ion. Note the group number gives the number of valence electrons contributed by each atom.

1A	2A	3A	4A	5A	6A	7A	8A	
Li	Be	B	C	N	O	F	Ne	
Na	Mg	Al	Si	P	S	Cl	Ar	Etc.

(If the charge is negative add electrons, and
if the charge is positive subtract electrons.)

Step 2: Write the skeleton structure of the molecule. The least electronegative atom will be central. Hydrogen is probably not central.

Step 3: Use two valence electrons to form each bond in the skeleton structure between the central and the outer atoms.

Step 4: Try to satisfy the octets (duet for H) of the atoms by distributing the remaining valence electrons as nonbonding electrons. It is usually best to start with the outer atoms.

Additional Rules

1 Thou shalt not violate the octet rule for C, N, O, and F. (C, N, O, F)

2. B and Be may have less than an octet because they are not very electronegative.

3. Third row elements or lower in the periodic table (ie P, S, Cl) may exceed the octet rule.

4. Always try to satisfy the octet rule first, then if electrons are left over, place the excess electrons on 3rd period atoms.

Formal Charges

1 Formal Charge = (Valence electrons) – (assigned electrons)
(on the free atom)

Assigned electrons = lone pairs + ½(the bond pairs)

In other words for formal charge purposes, an atom owns all the electronbs in the lone pairs on that atom, and the atom shares the electrons in bonds with the atom that it is bound to.

2. Sum of the formal charges must equal the overall charge. For neutral molecules the overall charge is zero.

3. If several structures exist, the best structures are those with the fewest formal charges and with any negative charges on the most electronegative atoms.

VSEPR structures.

A Lewis structure simply gives one the correct distribution of electrons, but says nothing about the shape of the molecule. A simple way to determine the shape is called VSEPR which stands for Valence Shell Electron Pair Replusion. This model assumes that the electrons distribute themselves about an atom to minimize repulsions between pairs of electrons.

Steps

1. Get a valid Lewis structure.

2. An effective pair of electrons in defined as either:
a) a lone pair - 2 electrons
b) a single bond pair - 2 electrons
c) a double bond - 4 electrons
d) a triple bond - 6 electrons

3. Count the number of effective electron pairs about an atom. These electrons will be arranged in the following geometries according to this number:

Effective Electron Pairs	2	3	4	5	6
Geometry	Linear	Trigonal Planar	Tetrahedral	Trigonal Pyramidal	Octahedral

The shape of the molecule only includes the central atom and the bonded atoms. That is the lone pairs determine the shape, but are not part of the shape. The shapes you neeed to know are on a separate page that shows the effect of lone pairs on the shape.

Determining polarity

Get a valid VSEPR structure

A molecule can be nonpolar in either of two ways:

A) All the bonds are nonpolar

B) Some bonds are polar and the bond vectors cancel out

A bond is polar if the difference in electronegativity between atoms is greater than about 0.6

Bond vectors are arrows that are drawn from the less electronegative atom to the more electronegative atom along the bond between the two atoms.

The length of a bond vector is proportional to the difference in electronegativity. (i.e. a larger difference means a larger length for the bond vector)

Bonds vectors are vectors so they have both a length and a direction in space.

A molecule can be polar only if it meets both of the following conditions:

A) It must have polar bonds

and B) The bond vectors do not cancel out

To determine if a molecule that has polar bonds is polar overall, add the combine the bond vectors according to the rules of vector addition. This means you must consider both the length and the direction in space. Vectors are added head to tail (i.e. move the tail of the second vector to the head of the first vector with out changing the directions of either vector. The line from the tail of the first vector to the head of the second vector is the vector sum. In pictures:

If the vector sum of all the bond vectors is zero, then the molecule is nonpolar

If the vector sum is not zero, then this resultant is the dipole moment. A dipole moment is a vector so it has a length and a direction.

Bond vectors that will cancel : A) Two equal vectors in opposite directions

B) Three equal vectors at 120º angles to each other

C) Four vectors arranged in a tetrahedral fashion.

Whitener's Rule: If a central atom has exactly one lone pair and polar bonds, the molecule is polar.