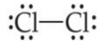
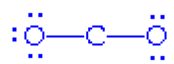
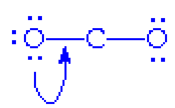
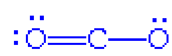
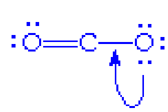
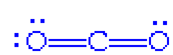
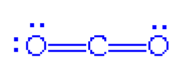
Lewis Structure Exercise

A Lewis structure shows how the valence electrons are arranged and indicates the bonding between atoms in a molecule. We represent the elements by their symbols. The shared electron pair is shown as a line/bond between the two atoms. All the other valence electrons are shown as dots or lines around the symbol of the element.

For Example: The Lewis structure for Cl_2 is 

Let us now see how to draw the Lewis structure for CO_2

Steps for drawing Lewis Structures	Example with CO_2
1. Sum the valence electrons of all the atoms. • For anions, add one electron for each negative charge. • For cations, subtract one electron for each positive charge.	The total number of valence electrons is 16 (4 from carbon and 6 from each oxygen).
2. Choose the least electronegative element (other than H) as the central atom. • For a molecule of type XY_n, X is always the central atom.	Choose carbon as the central atom since it is less electronegative and also follows the XY_n rule.
3. Use single bonds (lines) to connect the central atom to the surrounding atoms.	Attach the two oxygens to carbon by single bonds. O – C – O
4. Subtract 2 electrons for each bond from the original total number of electrons.	We subtract 4 electrons (2 for each bond) from 16 leaving 12 electrons to distribute to the remaining atoms.
5. Complete the octet for all outer atoms (other than H). Each bond to an atom will count as 2 electrons for that atom's octet.	Complete the octet for each of the oxygen atoms which uses the last 12 electrons. (We need to add 6 electrons to each oxygen.) 
6. Complete the octet for the central atom.	There are no more electrons, so we cannot add more to the central atom to complete its octet.
7. If you run out of electrons before the octet for the central atom can be completed, start forming multiple bonds until the central atom has a complete octet. When you form a multiple bond, remember to remove an electron pair from the outer atom.	Since carbon does not have an octet, form multiple bonds by taking the lone pairs.  becomes  The central atom is still electron deficient, so share another pair.  becomes 
8. Make sure the correct number of electrons has been used and that every atom's octet is complete. *The exceptions are atoms of group 2 and 3 which can have incomplete octets and atoms in period 3 or greater which can have expanded octets.*	4 bonds + 2 electron pairs equal 16 electrons. All atoms have an octet. 

Molecular Geometry – the Valence Shell Electron Pair Repulsion (VSEPR) Theory

The electron groups around the central atom repel each other and therefore prefer to be as far apart from each other as possible. This is the main idea of the VSPER theory. We can apply the VSEPR theory to predict the molecular shape/geometry of a molecule.

1. Draw the Lewis structure for the molecule in question.
2. Count the total number of electron groups on the central atom. Add the number of atoms bonded to the central atom and the number of lone pairs on the central atom – this is the total number of electron groups. Note that multiple bonds to <u>one</u> outer atom still count as <u>one</u> electron group.
3. The arrangement of the electron groups is determined by minimizing the repulsions between them.
4. Remember that lone pairs require more space than bonding pairs. Therefore, choose an arrangement that gives lone pairs as much room as possible.

The attached table shows the relationship between the number of electron pairs and the molecular geometry.

Polarity of a molecule

A covalent bond is polar if there is a difference in electronegativity between the bonded atoms. A molecule like HCl has a polar covalent bond since there is a difference in electronegativity between the two atoms (the difference is greater than 0.4 and less than 1.8). Thus HCl possesses a permanent dipole moment because the molecule has a distinct negative end and a distinct positive end. However, just because there is a polar bond present in a molecule does not necessarily mean that the molecule is polar. If all the dipoles in the molecule cancel each other out, then the molecule will be non-polar. For example, CO_2 has two polar bonds, but they point in opposite directions and cancel each other out.

Formal Charges

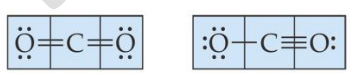
The formal charge of any atom in a molecule is the representation of electron distribution on the atom. *Remember that the formal charge does not represent the real charge on the atom*. It is a fictitious charge assigned to each atom that helps in finding the best Lewis structure for a molecule.

The best Lewis structure will

- Have the lowest possible formal charge on each atom
- Put the negative formal charge on the most electronegative atom (and a positive formal charge on the least electronegative atom)

<u>Calculating formal charges</u>

- Sum all the electrons in the lone pairs belonging to that atom
- Add to this half of the bonding electrons
- Subtract this total from the number of valence electrons for that atom to get its formal charge.



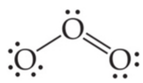
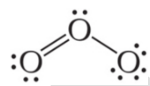
	O	C	O	O	C	O
Valence electrons:	6	4	6	6	4	6
−(Electrons assigned to atom):	6	4	6	7	4	5
Formal charge:	0	0	0	−1	0	+1

In the above example for CO_2, the Lewis structure on the Left is the better one as it places a formal charge of zero on each atom. Recall that the formal charges sum to zero for a molecule and to the charge for an ion.

Resonance

Sometimes one Lewis structure is not enough to describe a molecule completely. For example, ozone (O_3) can be represented by the following two structures:

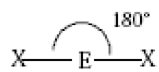
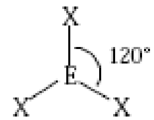
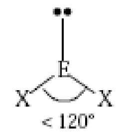
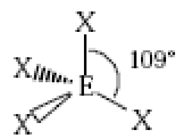
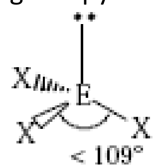
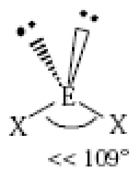
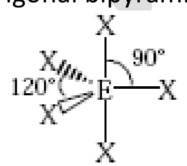
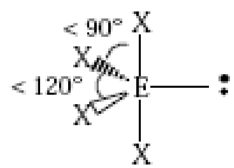
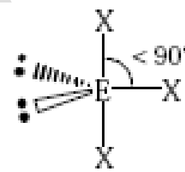
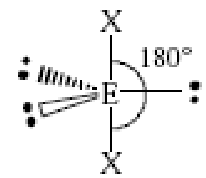
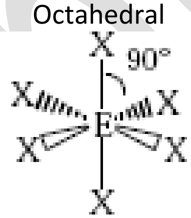
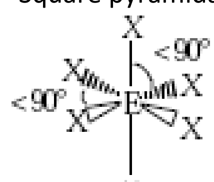
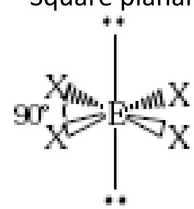
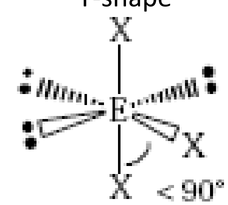
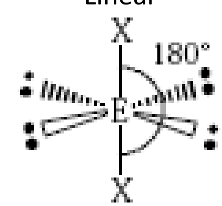
One might expect ozone to have one single bond and one double bond based on either of the above Lewis structures. However, experimentally it is found that both the bonds are equivalent and intermediate between a single and a double bond. Thus, the true structure of ozone is a resonance hybrid of the above two Lewis structures. We represent resonance by drawing the two structures with a double headed arrow between them. Remember that although we may draw two resonance structures, there is actually only one structure that is a hybrid of the two drawings – the molecule does not "flip" back and forth, but rather is permanently somewhere between the two structures. Each bond in ozone is a combination of one single and half a double bond.

 ↔ 

In the above example, both the Lewis structures are equivalent and contribute equally to the true structure of ozone. However, sometimes some of the Lewis structures are preferred over others (see the discussion on formal charges above). In that case, the preferred Lewis structure(s) contribute more to the overall structure of the molecule.

Hybridization

To explain molecular geometries, we assume that orbitals mix together to form new orbitals. This process of mixing atomic orbitals is called hybridization. The new orbitals are called hybrid orbitals. The number of hybrid orbitals formed will be equal to the total number of orbitals that are mixing together.

VSEPR Geometries						
Number of electron groups on the central atom	**Hybridization**	**0 lone pair on central atom**	**1 lone pair on central atom**	**2 lone pairs on central atom**	**3 lone pairs on central atom**	**4 lone pairs on central atom**
2	sp	Linear 				
3	sp^2	Trigonal planar 	Bent 			
4	sp^3	Tetrahedral 	Trigonal pyramidal 	Bent 		
5	sp^3d	Trigonal bipyramidal 	See-saw / sawhorse 	T-shape 	Linear 	
6	sp^3d^2	Octahedral 	Square pyramidal 	Square planar 	T-shape 	Linear 

Lewis Structures: Work Sheet **Name ________________________**

Make molecular models of the compounds listed in the table below and complete the table.

Molecular Formula	Lewis Structure	Number of electron groups on central atom	Number of lone pairs on central atom	Molecular geometry	Bond angle(s)	Polar? Yes or No	Hybrid-ization
H_2CO							
ClF_3							
H_2O_2							
OCS							
ClO_2 -						N/A (ionic)	
N_3^-						N/A (ionic)	

Molecular Formula	Lewis Structure	Number of electron groups on central atom	Number of lone pairs on central atom	Molecular geometry	Bond angle(s)	Polar? Yes or No	Hybrid-ization
PF_3							
XeF_4							
BH_3							
ClF_2^+						N/A (ionic)	
SO_2							
HCN							

Lewis Structures: Post Lab Questions **Name** ________________________

1. For the following molecules/ions **1)** Draw all possible resonance Lewis structures.
2) Assign formal charges for all atoms in each resonance structure.
3) Circle the favored resonance form; if all forms are equivalent, circle none.

a) N_2O (Connectivity is N-N-O)

b) CO_3^{2-}

c) CH_3COOH (Both O are connected to Second C, last H attached to O)

2. The following are the two possible Lewis structures for $C_2H_2F_2$. Will both of them have the same dipole moment? Explain clearly.