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Experiment #10: Geometrical Structure of Molecules and Ions using Molecular Models

In Chemistry 1A, you are introduced to four theories involving molecular models: Lewis dot structures, Valence Shell Electron Pair Repulsion (VSEPR) Theory, Valence Bond (VB) Theory, and Molecular Orbital (MO) Theory. This experiment combines the first three theories. It gives you an opportunity to predict the Lewis dot two-dimensional structures on paper, physically build the three-dimensional models using ball and stick pieces, determine the expected angles and shapes using VSEPR Theory, and identify the hybridized orbitals and number of sigma (σ) and pi (π) bonds using VB Theory.

Lewis dot structures are two-dimensional models that use all of the valence electrons available. Covalent bonds form when nonmetals combine to share electrons, creating single, double, or triple bonds. Ions are always represented inside brackets with the overall charge indicated on the outside upper right. For ionic compounds, you separate the cation and anion, keeping both inside their own brackets. Lewis structures give you a great amount of information such as bond types, resonances, structural isomers, formal charges, and dipole arrows between atoms. Most elements follow and prefer the octet rule; exceptions include: (1) octet deficient (H, Be, B) atoms, (2) an odd number of total electrons prevent the possibility of an octet for all atoms, and (3) expanded octets possessing 10 or 12 electrons around a central atom, beginning with period three and higher elements. The BEST Lewis structures follow the octet rule and minimize formal charges.

Valence Shell Electron Pair Repulsion (VSEPR) Theory states that bonds and lone pairs are regions of high electron density in an atom that repel each other until they get as far apart as possible. This effect determines the atom's three-dimensional geometry and bond angles. Two regions will be 180° apart; three regions will be 120° apart; and four regions will be 109.5° apart. Expanded octets which are not pictured here include the trigonal bipyramidal electronic geometry that has five regions (2 axial positions 180° apart from each other and 90° from the 3 equatorial positions that are 120° apart from each other) and the octahedral electronic geometry that has six regions (all 180° and 90° apart from each other as in an x, y, z three-dimensional axis).

The Valence Bond (VB) Theory is also three-dimensional and has the same angles as predicted by VSEPR Theory. In addition, VB Theory promotes the notion that these shapes appear because the atomic orbitals have become hybridized. Hydrogen keeps its simple *s* orbital. Atoms with two regions now possess two identical *sp*-hybridized orbitals, three regions have 3 sp^2 hybrid orbitals, 4 regions become sp^3 hybridized, five regions are sp^3d hybridized, and six regions form sp^3d^2 hybrid orbitals. All bonds also have a sigma (σ) bond that directly overlaps. Multiple bonds possess sigma and pi (π) bonds that indirectly overlap perpendicular to the hybridized orbitals, where double bonds include 1 sigma and 1 pi bond, and triple bonds include 1 sigma and 2 pi bonds.

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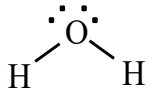
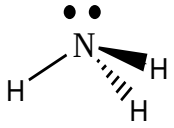
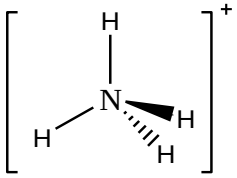
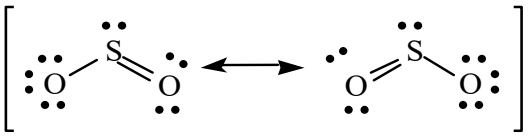
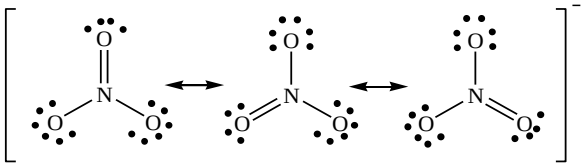
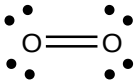
Partial VSEPR Table (look to your book or notes for expanded octets)

# of areas	# of bonds	# of lone pairs	Geometry and bond angles	Example
4	2	2	Angular or bent (~109.5°)	
4	3	1	Trigonal Pyramidal (~109.5°)	
4	4	0	Tetrahedral (109.5°)	
3	2	1	Bent (~120°)	 2 resonance forms
3	3	0	Trigonal Planar (120°)	 3 resonance forms
2	2	0	Linear (180°)	H–C≡N:
	1	any	Linear (Must have three or more atoms to form an angle.)	

Notice the convention for drawing bonds in 3-D space, where:

- the wedge (◣) represents a bond coming out of the paper, and
- the dash (·····) represents a bond going behind the paper.

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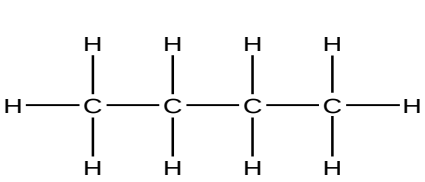
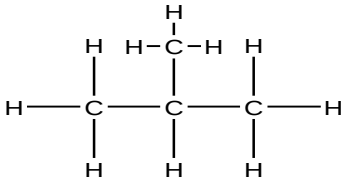
Do not confuse resonance structures with structural isomers. Resonance structures contain atoms in the same position but electrons are delocalized throughout. Structural isomers are molecules having the same chemical formula but different connectivity of the atoms. For example, two isomers are possible for a molecule with the formula C_4H_{10}:





Procedure

For each of the ions or molecules listed:

A. Draw the Lewis dot structure. For those with resonance, draw all possibilities. When requested, draw all the different structural isomers. Remember that single bonds can twist, but multiple bonds cannot.

B. Use the model kit to build the structure.
   - The white atoms represent hydrogen and can form one bond each.
   - The black, blue, and red atoms represent atoms that desire a complete octet.
   - Use short sticks for nonbonded electron lone pairs
   - Use long sticks for single bonds.
   - Use multiple springs for double and triple bonds.
   - Use purple atoms for trigonal bipyramidal electron geometry
   - Use silver atoms for octahedral electron geometry

C. For each central atom in the structure, determine the number of areas of electron density that lie directly on that atom. An area of electron density may be:
   - a lone (nonbonding) pair or dot that lies on the atom in question
   - a single bond
   - a double bond
   - a triple bond

D. Fill in the empty spots on the table. Assign bond angles, formal charges, dipole arrows for polar bonds, and molecular geometries. Determine the polarity of the species, atomic and hybridized orbitals, and number of pi bonds.

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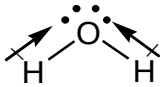
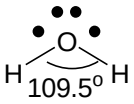
Complete the following table for the indicated species:

Substance	**H_2O**	**HF**	**O_2**	**CO**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero	 (does NOT need to be bent at this point!) formal charge $_O = 0$ formal charge $_H = 0$			
Name the electronic geometry around central atom(s)	Tetrahedral			
Give hybridization for central atom(s)	sp^3			
Name the shape around central atom(s)	Bent (or angular)			
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?	2 σ and 0 π bonds			
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?	polar molecule			

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Complete the following table for the indicated species:

Substance	**NH_4^{+1}**	**Na_2S**	**SO_3**	**ClO_2^-**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero				
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				

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Complete the following table for the indicated species:

Substance	**SO_3^{-2}**	**CH_2O**	**CO_2**	**SCN^-**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero				
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				

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Complete the following table for the indicated species:

Substance	**$C_2H_2Br_2$**	**NF_3**	**CH_2Cl_2**	**CH_3OH**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero				
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				

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Complete the following table for the indicated species:

Substance	**C_6H_6 (ring)**	**S_8**	**PO_4^{-3}**	**C_3H_8O**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero				
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				

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Complete the following table for the indicated species:

Substance	**NO_3^-**	**NO_2**	**H_2O_2**	**C_2H_2**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero				
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				

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Complete the following table for the indicated species:

Substance	**A: $C_2H_4O_2$**	**B: $C_2H_4O_2$**	**C_2H_6**	**BaO**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero	Draw one structural isomer with C–C bond that has one C connected to 3 H and the other to 2 O. This is acetic acid	Draw a new structural isomer keeping all formal charges = 0. More than 5 isomers are possible		
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				

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Complete the following table (the central atom for each species has an expanded octet):

Substance	**I_3^-**	**ICl_5**	**SF_6**	**$XeOCl_2$**
a) Draw the best Lewis structure(s), resonances, and structural isomers if any b) In your structure above, indicate polar bonds with dipole arrows toward the more electronegative atom c) Include formal charges if they are not zero				
Name the electronic geometry around central atom(s)				
Give hybridization for central atom(s)				
Name the shape around central atom(s)				
Show 3-D sketch of the structure and label all bond angles				
How many sigma bonds? How many pi bonds?				
Is the substance an ionic compound, a polar molecule, a nonpolar molecule, or a polyatomic ion?				