

Names: _____

Molecular Modeling Report Form

These pages replace the Molecular Model Lab, pp. 97-103, of the Chemistry 108 Experiments Lab Manual. Complete the following modeling related exercises and include the names of all group members, who contributed to the work, on the form.

The first column lists formulas for a number of compounds. The bonding type is to be determined for these compounds using differences in their respective electronegativity values (refer to the in class information). The second column is for the electronegativity difference, the absolute value of the difference in electronegativity between the 2 different atoms in the compound, $|EN_2 - EN_1|$.

The third column is for the average electronegativity of the two atoms, $(EN_1 + EN_2)/2$.

Compound	$EN_1 - EN_2$	$\frac{EN_1 + EN_2}{2}$	Bonding Type
HF			
HCl			
HBr			
HI			
CsF			
NaF			
CaO			
BaO			
NH ₃			
CH ₄			
CCl ₄			
H ₂ O			
N ₂ O			
SO ₂			
H ₂			
O ₂			

Construct a plot of electronegativity difference (y-axis) versus average electronegativity (x-axis) on the blank graph that follows on this page. Write the element or compound formula next to each data point.

Briefly explain: Are there any patterns in the graph? Did certain element or compound types clump together? Which bonding type is represented by each group? Complete the fourth column of the table on the first page.

You will digitally build, model, and explore various structures & shapes of covalently bonded molecules using an on-line computational program. Below is a general scheme for 4 of the most commonly bonded elements that are found in molecules of all living organisms. Complete the table for the electronic and molecular shapes associated with the bonding patterns using the information presented in class.

Symbol	Valence electrons	Number of Bonds	Types	Shape	
				electronic	molecular
C	4	4	4 single		
		4	2 single + 1 double		
		4	1 single + 1 triple		
H	1	1	1 single		
O	6	2	1 double		
		2	2 single		
N	5	3	3 single		
		3	1 single + 1 double		
		3	1 triple		

You will use MolView (<http://molview.org>), an open source, highly intuitive, interactive molecular modeling, computational, visualization program. Take a tour of MolView:


<https://www.youtube.com/channel/UCRP9nXCC59TMIqc-bk1mi3A>


Open the MolView page (<http://molview.org>) and click on **Get Started**.

The search and drawing features will be used to access & build 3-D molecules and to relate them to Lewis structures in the process. Read through the general description given in the **Drawing structural formulas** Tab. If you know the name of the illustrated chemical formula, the search function can be used. Complete the Lewis structures in the table, which will correspond to the displayed formulas if drawn correctly.

OPTIONAL: Using the models, draw 3-D line drawings in the table using the following convention.

Line: In the plane of the paper: ———

Wedge: Coming forward, in front of the plane of the paper: 

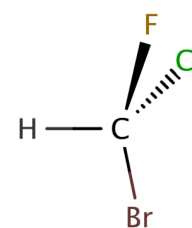
Dash: Going backward, behind the plane of the paper: 

For example: The 5 atoms in the CHFCIBr molecule are in the following positions:

in the plane of the paper __H__ __C__ __Br__

in front of the plane of the paper __F__

behind the plane of the paper __Cl__



Report Form – Molecular Models

Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	3 Dimensional Drawing	Resonance (Yes or No)
H ₂ O		<pre> O / \ H H </pre>				Polar		No
NH ₃		<pre> H H H - N - H </pre>				Polar		No
CH ₄		<pre> H H H - C - H </pre>						No
C ₂ H ₄		<pre> H H H H H - C - C - H - H </pre>	Around each C	Around each C	C-H C-C	Non-Polar		No
HCN		<pre> H C N H - C - C - N </pre>	Around C	Around C	H-C C-N	Polar		No
C ₂ H ₂		<pre> H C C H H - C - C - H - H </pre>	Around each C	Around each C	C-H C-C			No
SO ₃		<pre> O S O O - S - O - O </pre>				Non-Polar		Yes

Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	3 Dimensional Drawing	Resonance (Yes or No)
CBr_4		<pre> Br Br Br — C — Br Br Br </pre>						No
CO_2		<pre> O C O O C O </pre>						Yes
H_2S		<pre> S / \ H H </pre>						No
NF_3		<pre> F N F F F </pre>						No
SO_2		<pre> S / \ O O </pre>				Polar		Yes
CH_3OH		<pre> H C O H H C O H H H </pre>	Around C Around O	Around C Around O	C-H C-O O-H	Polar		No
$(\text{NO}_3)^-$		<pre> O N O O O </pre>				Polyatomic Ion		Yes

Chemical Formula	# Valence e's in Molecule	Lewis Structure	Name of VSEPR Arrangement (Geometry)	Name of Shape (Molecular Geometry)	Bond (Polar or Non-Polar)	Molecule (Polar or Non-Polar)	3 Dimensional Drawing	Resonance (Yes or No)
N_2		$\begin{array}{ccc} & N & \\ & & \\ N & & \end{array}$						No
$(NH_4)^+$		$\begin{array}{ccc} & H & \\ & & \\ H & N & H \\ & & \\ & H & \end{array}$				Polyatomic Ion		No
PBr_3		$\begin{array}{ccc} & P & Br \\ & & \\ Br & & \\ & & \\ & Br & \end{array}$				Polar		No
$(NO_2)^-$		$\begin{array}{ccc} O & & O \\ & N & \\ & & \end{array}$				Polyatomic Ion		Yes
$(CO_3)^{2-}$		$\begin{array}{ccc} O & & O \\ & C & \\ O & & \end{array}$				Polyatomic Ion		Yes
CH_2O		$\begin{array}{ccc} & O & \\ & & \\ H & C & H \end{array}$						No