Name: ________________
Class: ________________

VSEPR Theory Worksheet

Warm-Up Questions:

Watch the Khan Academy videos on VSEPR theory.

1) Carbonate, CO_3^{-2}, is a common polyatomic ion found in various materials from eggshells to antacids. Draw the Lewis structure of CO_3^{-2} and assign formal charges.

2) What is its electron domain geometry?

3) What is its molecular geometry?

Example #1:

Draw the Lewis structure for $SeCl_2$. Then, determine the number of electron domains and predict the electron domain and molecular geometry of $SeCl_2$ using the VSEPR model. Hint: Determine which atom is the central atom and don't forget about the octet rule!

- Lewis structure:

- # of electron domains (including lone pairs):

- Electron domain geometry:

- Molecular geometry:

Computational Exercise #1:

Lewis Structure with predicted bond angles of $SeCl_2$ using the VSEPR Model:	Optimized geometry of $SeCl_2$ using Maestro:

Number of electron domains in $SeCl_2$:

Electron domain geometry:

Molecular geometry:

Predicted Cl–Se–Cl bond angle:

Calculated Cl–Se–Cl bond angle:

Example #2:

For each molecule below, (i) draw the Lewis structure with nonbonding electrons, (ii) determine the number of nonbonding lone pairs and bonding pairs on the central carbon atom, and (iii) predict the electron domain and molecular geometries using the VSEPR model.

	Lewis Structure	# of Nonbonding Lone Pairs on Carbon(s)	# of Bonding Pairs on Carbon(s)	Electron Domain Geometry	Predicted Molecular Geometry
HCN					
C_2H_4					
CH_3F					

Computational Exercise #2:

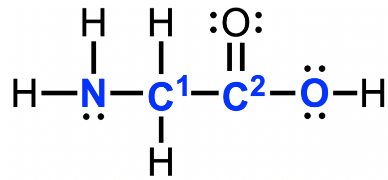
For each molecule from Example #2, optimize each of their geometries using the DFT methods listed below. Then, determine all of the bond lengths and angles in each molecule. Check if your calculated measurements match the predicted values from your proposed molecular geometries based on the VSEPR method.

- Theory: B3LYP-D3
- Basis set: 6-31G** (6-31GSS)

	Optimized Geometry using Maestro	**Bond Angles**	**Bond Distances**	**Predicted Molecular Geometry**
HCN				
C_2H_4				
CH_3F				

Example #3:

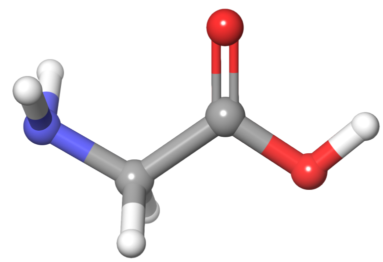
The Lewis structure for the simplest amino acid, glycine, or $H_2NCH_2CO_2H$, is shown below. Predict the local geometry for the nitrogen atom, the two carbon atoms (labeled as C1 and C2), and the oxygen atom with a hydrogen atom attached. These atoms are also bolded in blue.



	# of Nonbonding Lone Pairs	# of Bonding Pairs	Electron Domain Geometry	Predicted Molecular Geometry
N				
C^1				
C^2				
O				

Computational Exercise #3:

Using the optimized structure of glycine, determine the following bond angles and see if your molecular geometry predictions from the VSEPR model match the calculated structure.



	Bond Angle	Predicted Molecular Geometry
N	H–N–H angle:	
C^1	N–C–C angle: N–C–H angle:	
C^2	O–C–O angle:	
O	H–O–C angle:	

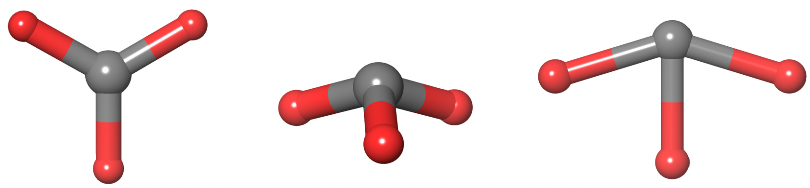
Analysis:

Individual Exercises

Part A: For each molecule below, (i) draw the Lewis structure with nonbonding electrons, (ii) determine the number of nonbonding lone pairs and bonding pairs on the central atom highlighted in blue, and (iii) predict the electron domain and molecular geometries using the VSEPR model.

	Lewis Structure	# of Nonbonding Lone Pairs on Central Atom	# of Bonding Pairs on Central Atom	Electron Domain Geometry	Predicted Molecular Geometry
H_3CNH_2					
BH_3					
ClF_3					

Part B: Shown below are ball-and-stick representations of three different AB_3 molecules where all "A" atoms are grey and all "B" atoms are red. Match the three molecules from Part A to the closest ball-and-stick representation and explain your reasoning. Remember to focus on the geometries around the *central atom*.



Molecule A ***Molecule B*** ***Molecule C***

- Molecule A is ___________ because…

- Molecule B is ___________ because…

- Molecule C is ___________ because…

Part C: For each molecule from Part A, optimize each of their geometries using the DFT methods listed below. Then, determine all of the bond lengths and angles in each molecule. Check if your calculated measurements match the predicted values from your proposed molecular geometries based on the VSEPR method.

- **Theory:** B3LYP-D3
- **Basis set:** 6-31G** (6-31GSS)

	Optimized Geometry using Maestro	Bond Angles	Bond Distances	Predicted Molecular Geometry
H_3CNH_2		H–N–C angle:	N–H bond: C–N bond:	
BH_3		H–B–H angle:	B–H bond:	
ClF_3		Cl–F–Cl angle:	F–Cl bond:	