Experiment 10:
Molecular Geometry Visualization

Safety First!

Potential Hazards

- **None**

Waste Disposal

- **None**

Experiment Objective(s):

- Students will draw Lewis structures and use VSEPR theory to visual molecules in 3 dimensions.
- Students will draw small molecules in *GaussView* and set up basic quantum chemical calculations using the Gaussian program.
- Students will use the GaussView program to view optimized bond lengths, bond angles and dihedral angles, as well details of dipole moments.

Learning Objectives: In this lab you will begin to learn how to use basic tools of computational/quantum chemistry to approximate a molecular geometries and electronic distribution. The modeling program will allow you to visualize the model in 3-dimensions and view the magnitude and direction of the polarity. It will also allow you to compare the energies of geometric isomers of molecules to determine preferred shapes.

Students will use a state-of-the-art computational program, Gaussian 09, with its beginner-friendly graphical user interface GaussView 5.0, to model and analyze the structure and properties of different molecules. Calculations will include geometry optimization at simple HF/3-21G level, single-point calculations, and calculations of harmonic frequencies. The frequency analysis will provide detailed information of vibrational spectrum of molecule and displacement of each vibrational mode that will help student understand the vibrational spectroscopy. Students will be able to visualize the polarity of small molecules by calculating the dipole moment.

Background:

Lewis Theory and Valence Shell Electron Pair Repulsion (VSEPR) Theory are two simple but very powerful tools that chemists use to visualize molecular shapes in three dimensions. These two theories work hand in hand with each other; Lewis theory giving the assignment of the electrons to their appropriate atoms within a molecule and VSEPR theory creating the three dimensional space in which these bonded atoms and electron groups can exist.

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Although these two theories do not require the sophisticated computational calculations involve in this laboratory exercise, we will use this program to explore and verify the conclusions drawn by Lewis and VSEPR theories. This program will also allow us to visualize molecules in various forms in three dimensions.

Procedures:

Come to lab with **2 copies** of your pre-lab. You can either write the structures out twice, or make a photocopy. You will need one copy to turn in, and the other copy to use as you work with your partner to build molecules.

For this lab, please work in PENCIL!

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Pre-lab Questions

For this lab, you must have TWO COPIES of the pre-lab – one to turn in, and one to work from.

Draw Lewis structures for each of the following molecules or ions:

1. $BeCl_2$	9. BrF_3
2. BF_3	10. I_3^-
3. O_3	11. SF_6
4. CH_4	12. IF_5
5. PCl_3	13. XeF_4
6. H_2O	14. CH_3CH_2OH
7. PF_5	15. C_6H_{12} (cyclic – the carbons form a ring)
8. SF_4	

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2nd copy (you may also photocopy your answers)

Draw Lewis structures for each of the following molecules or ions:

1. $BeCl_2$	9. BrF_3
2. BF_3	10. I_3^-
3. O_3	11. SF_6
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Procedures:

Equipment and Chemicals

- **Pauling Cluster in Wishnick Hall (WH210).**
- **This worksheet.**
- **Your laboratory notebook.**

Follow the procedures outline on the following pages..

<u>Problem 1:</u> Looking at the simplest molecule, H_2

STEP 1. Login.

1.1. Find "Pauling Cluster Lab Users Account" or enter "pclu" into username box (Figure 1.1*a*).

1.2. Enter password. Your Instructor or TA will provide password (Figure 1.1*b*).

(***a***) 

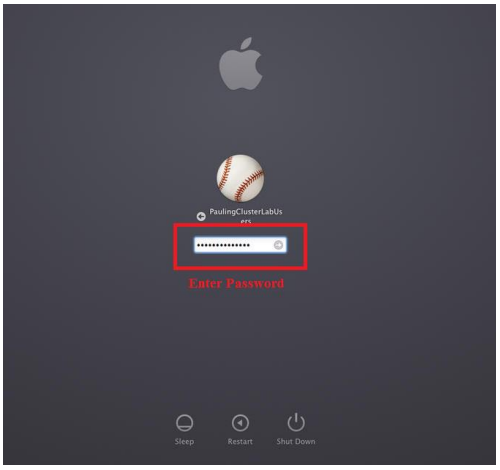
(***b***) 

Figure 1.1.

STEP 2. Run GaussView 5.0

2.1. Create a folder named "H2" on the Desktop. You will do calculations in this folder. Open Finder (Figure 2.1*a*).

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(*a*) 

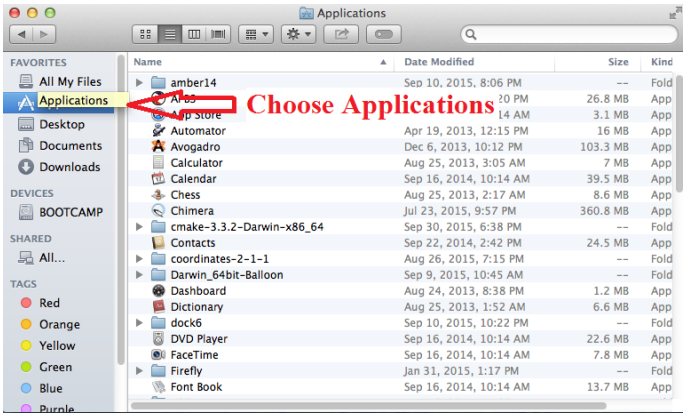
(*b*) 

Figure 2.1

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2.2. Open Applications. When you open Finder, choose Applications tab on the left sidebar (Figure 2.1*b*).

2.3 Find GaussView_Launcher in Applications, double click to run. If it doesn't start, click right button and choose "Open with" and then choose "Terminal.app" (Figure 2.2).

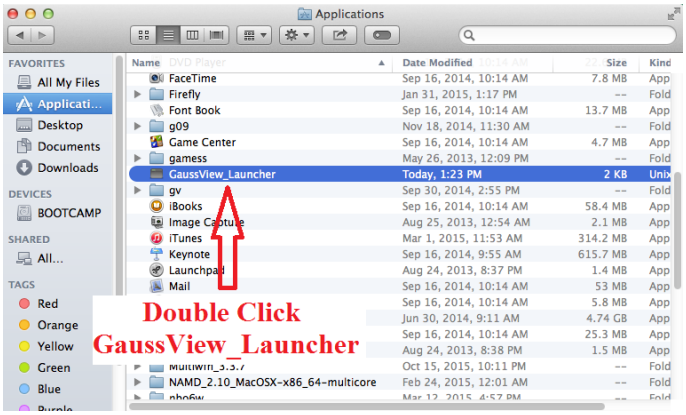

Figure 2.2

STEP 3. Getting familiar with GaussView 5.0

After you run GaussView_Launcher, it will open four windows (Figure 3.1):
#1 is main GaussView interface that has many options to build your molecule.
#2 is View Window that shows your current molecule and calculated properties.
#3 is tips window, and you can close it.
#4 is startup process, and you can close it after you open GaussView.

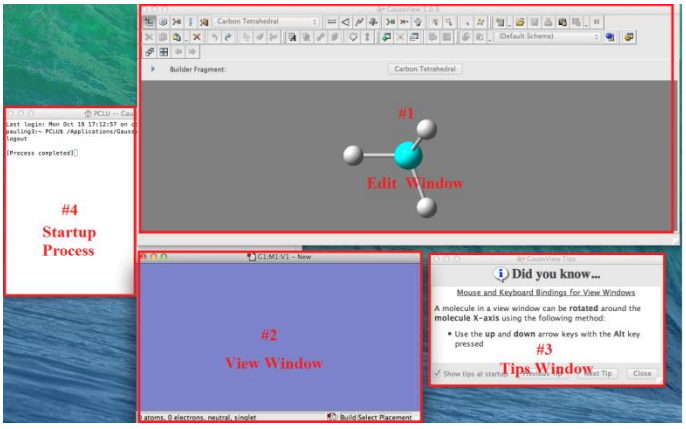

Figure 3.1

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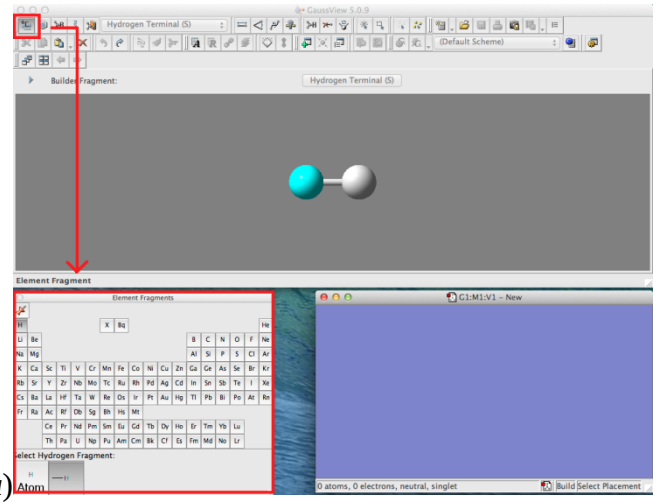
STEP 4. Geometry Optimization.

4.1 Click the button on the up-left corner to open periodic table. Choose atom or fragment. Next, click on View Window to build molecule (Figure 4.1*a*).



(***a***) (***b***)

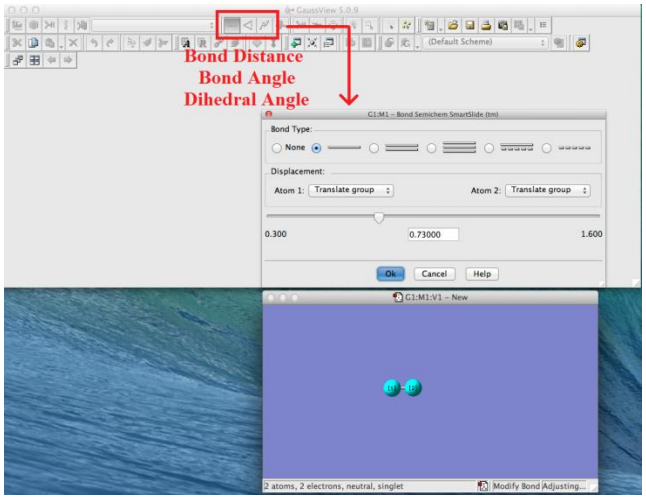


Figure 4.1

4.2 There are three tools (working with bond distance, bond angle, and dihedral angle, respectively) to edit your molecule. We choose the first button to set bond length equals to 0.74, and then click "OK" (Figure 4.1*b*).

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4.3 Choose “Calculation” on the top of window and choose “Gaussian Calculation Setup…”. It will pop up a new window to specify the setting of the calculation (Figure 4.2).

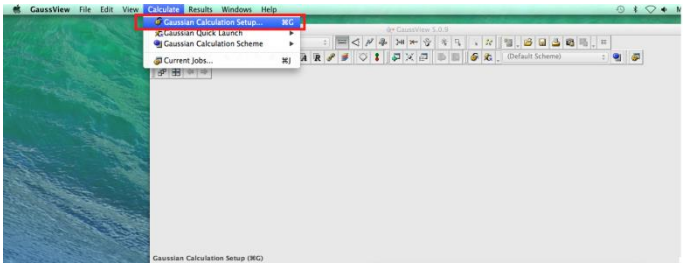

Figure 4.2

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4.4 In "Gaussian Calculation Setup" panel, we first specify "Job Type" to "Opt+Freq", which combines a geometry optimization step and frequency analysis together (Figure 4.3*a*).
(*Hints for other keywords: "Energy" is for single point calculation. "Optimization" and "Frequency" are for single geometry optimization and frequency analysis, respectively. "IRC" is for intrinsic reaction coordination calculation. "Scan" is for potential energy surface scan calculation." Stability" is for test the stability of wavefunction with respect to relaxing various constraints. "NMR" is for NMR chemical shielding calculations.*)

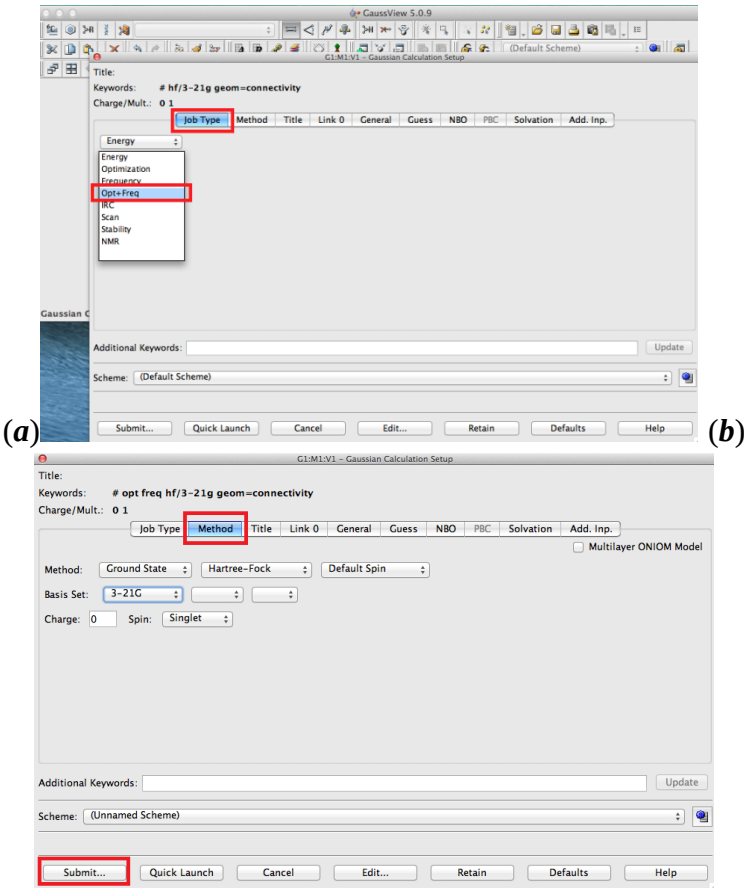

Figure 4.3

4.5 Now we specify the method we use for our calculation. We choose "Ground State" of "Hartree-Fock" method with "Default Spin". Basis set is "3-21G" without any more functions. Our molecule is neutral and all electrons are paired. Hence, the charge is "0" and Spin is "Singlet" as default. After that, we click "Submit…" to run the calculation (Figure 4.3*b*).

4.6 Save input file for our molecule into the folder where calculation runs (Figure 4.4*a*). For example, we created a folder on Desktop called "H2", so the path to "H2" is: "/User/PCLU/Desktop/H2/". The input file should be named as "H2.com" (Figure 4.4*b*). Once save the input file, choose "OK" to submit calculation (Figure 4.5).

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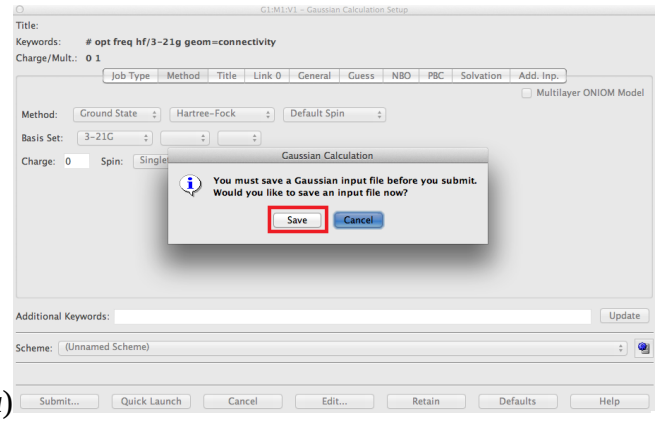

Figure 4.4

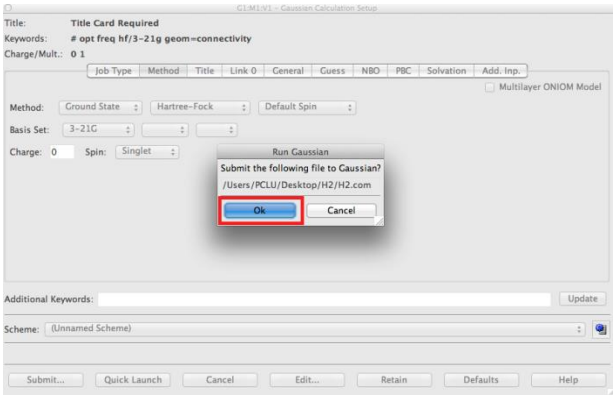

Figure 4.5

4.7 Check calculation status. In "Calculation" options, we choose "Current Jobs…" to see the status of submitted calculation (Figure 4.6*a*). It will open a window showing which calculation is running or waiting. It also can manage the submitted calculation (Figure 4.6*b*).

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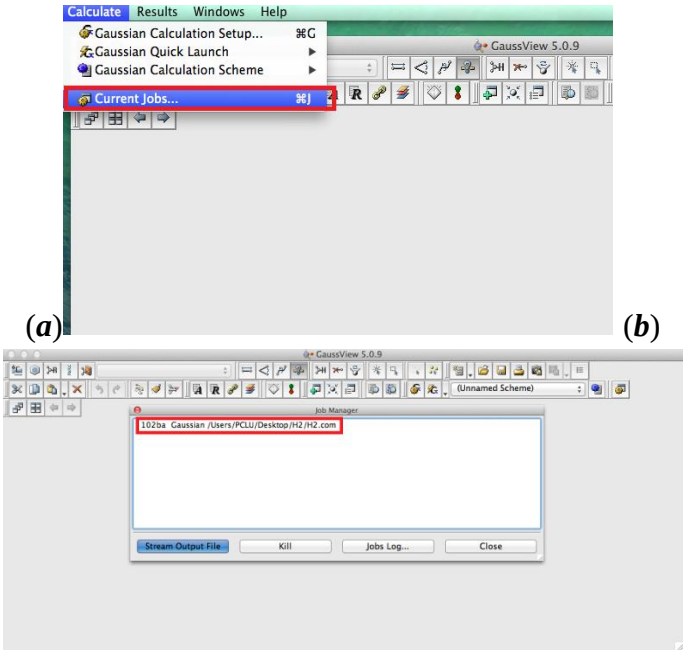

Figure 4.6

4.8 When the calculation finished, GaussView will pop up a window to show the output file. We choose the checkpoint file "*chk" to visualize calculation results (Figure 4.7).

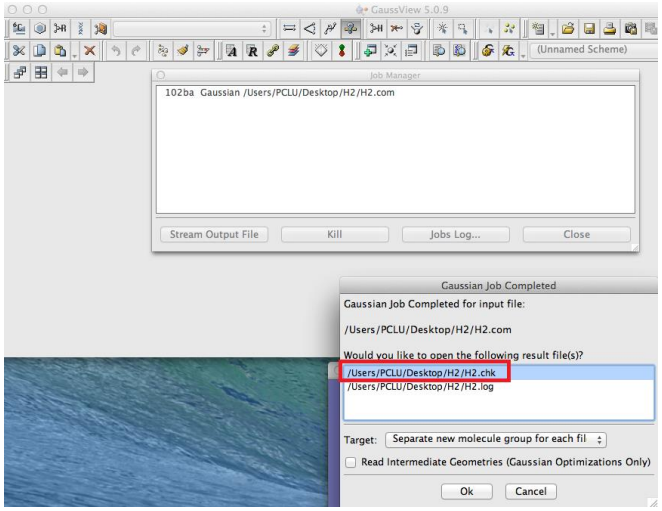

Figure 4.7

STEP 5. Calculation Results.

5.1 Choose "Results" on the top of window and choose "Summary" (Figure 5.1*a*). It will show basis results of your molecule, such as "Total Energy" and "Dipole Moment" (Figure 5.1*b*).

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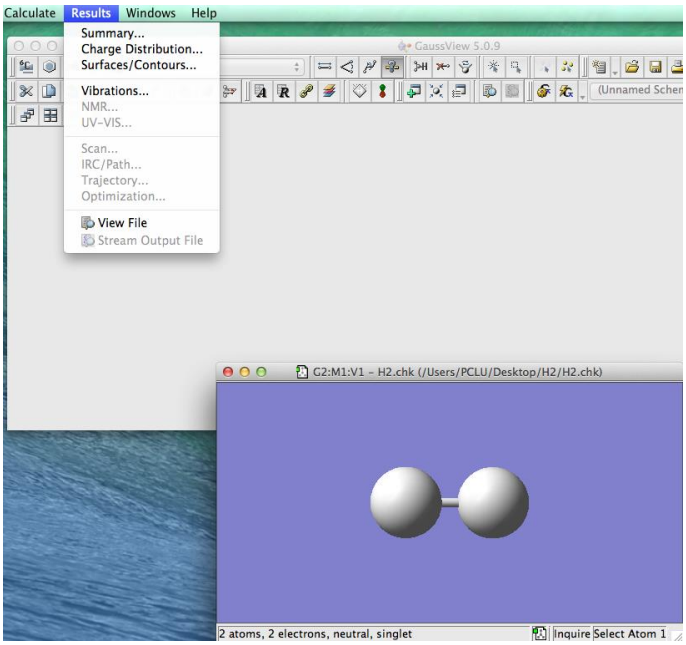
(*a*) 

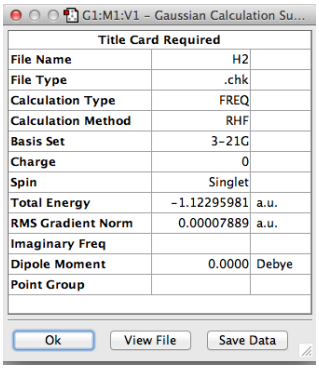
(*b*) 

Figure 5.1

5.2 In "Results" option, choose "Charge and Distribution…" to see charge distribution of your molecule. Check "Show Numbers", GaussView will label charges on atoms (Figure 5.2).

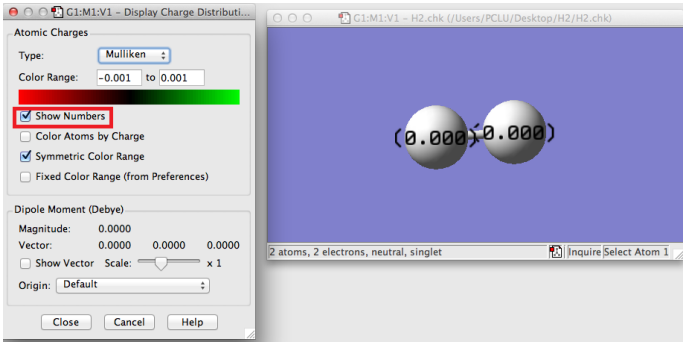


Figure 5.2

5.3 Also, in the same window (see Figure 5.2), click on "Show Vector" and use the scale slider to visualize the direction of the molecular dipole moment (polarity).

Experiment 10

Name_____ **Partner(s)**_____

Part A: Follow the procedure described for building H_2 to build the following molecules. Sketch their 3-D representation and recode their bond angles and polarities in units of Debye.

Molecule	Lewis Structure	Electron Group Geometry	Molecular Geometry	Sketch	Bond Angle	Molecular Polarity Dipole Moment (Debye)
$BeCl_2$						
BF_3						
O_3						

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Name_____ **Partner(s)**_____

Part B: Follow the procedure described for building H_2 to build the following molecules. Sketch their 3-D representation and recode their bond angles and polarities in units of Debye.

Molecule	Lewis Structure	Electron Group Geometry	Molecular Geometry	Sketch	Bond Angle	Molecular Polarity Dipole Moment (Debye)
CH_4						
NH_3						
H_2O						

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Name_____ **Partner(s)**_____

Part C: Follow the procedure described for building H_2 to build the following molecules. Sketch their 3-D representation and recode their bond angles and polarities in units of Debye. For geometric isomers, also record the total energy (in atomic units, a.u.) to verify the lowest energy conformation.

Molecule	Lewis Structure	Electron Group Geometry	Molecular Geometry	Sketch	Bond Angles	Molecular Polarity Dipole Moment (Debye)	Energy
PF_5							
SF_4 Tetra-hedral							
SF_4 See-saw							
SF_4 Trigonal-pyramidal							

Experiment 10

Name_____ **Partner(s)**_____

Part C (continued)

Molecule	Lewis Structure	Electron Group Geometry	Molecular Geometry	Sketch	Bond Angles	Molecular Polarity Dipole Moment (Debye)	Energy
ClF_3 T-shaped							
ClF_3 Trigonal planar							
I_3^-							

Experiment 10

Name_____ **Partner(s)**_____

Part D: Follow the procedure described for building H_2 to build the following molecules. Sketch their 3-D representation and recode their bond angles and polarities in units of Debye.

Molecule	Lewis Structure	Electron Group Geometry	Molecular Geometry	Sketch	Bond Angles	Molecular Polarity Dipole Moment (Debye)
SF_6						
BrF_5						
XeF_4 Square planar						
XeF_4 Trigonal pyramidal						

Experiment 10

Name_____ **Partner(s)**_____

Part E: Follow the procedure described for building H_2 to build the following molecules. Sketch their 3-D representation and recode their bond angles and polarities in units of Debye.

Molecule	Lewis Structure	Electron Group Geometry	Molecular Geometry	Sketch	Bond Angles	Molecular Polarity Dipole Moment (Debye)
CH_3CH_2OH						
C_6H_{12}						

Comments and observations.

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Post-Lab Questions

(I think we said they would turn this lab in at the end of class, so I did not include any post-lab questions. If we still want to have questions that they answer before they leave lab, I can add some.)