

Name: _____

Lab Section: _____

Chemistry 111 Lab Molecular Modeling Report Sheet

PART I

Table I.1- WebMO functions














Icon	Function
	
	
	
	
	
	
	
	
	
	
	
	
	

Table I.2- Water geometry

Method	O-H Bond Length (Å)	Bond Angle (°)
Idealized Geometry		
Mechanics		
Mopac calculation		
Experimental- water (<i>l</i>)	0.970	106.000
Experimental- water (<i>g</i>)	0.957	104.474

PART II- WHAT CONTROLS BOND LENGTH?

Table II.1- Control of Bond Length

Formula	Lewis Structure	Bond lengths
CH ₄		C-H
CH ₃ F		C-F
CH ₃ Cl		C-Cl
CH ₃ Br		C-Br
CH ₃ OH		C-H
		O-H
CH ₃ NH ₂		C-H
		N-H
CH ₃ CH ₃		C-C
CH ₂ CH ₂		C-C
CHCH		C-C

Part II Questions:

II.1 What are the two factors that control bond length?

II.2 Which of these has the largest effect on bond length?

II.3 Given your ideas, design a molecule that contains specific bonds you have not yet measured. For example, you could make a molecule that contains an S-F bond, or a P-Cl bond. Predict the bond length and then test your prediction by building and optimizing a model in WebMO.

Formula	Lewis Structure	Predicted Bond Length	Measured Bond Length
		Which bond: Length:	

PART III- WHAT CONTROLS BOND ANGLE?

Table III.1- Control of bond angle via number of structural electron pairs

Formula	Lewis Structure	# of Structural Pairs	Bond Angle
CH ₃ CN		on central C	C-C-N
BF ₃		on B	F-B-F
CH ₂ O		on C	H-C-H
CH ₄		on C	H-C-H
PF ₅		on P	F-P-F
SF ₆		on S	F-S-F

Table III.2- Control of bond angle via number of lone electron pairs

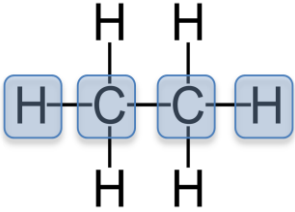
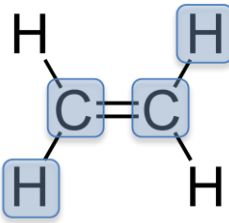
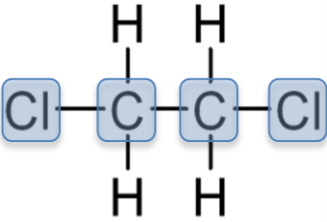
Formula	Lewis Structure	# of Structural Pairs	# of Lone Pairs on Central Atom	Bond Angle
CH ₄		on C		H-C-H
NH ₃		on N		H-N-H
H ₂ O		on O		H-O-H

Part III Questions:

- III.1 Does the number of structural pairs on the central atom control bond angles around that atom?
- III.2 Compare BF₃ and CH₂O. Each has a central atom with 3 structural pairs, but the C in CH₂O has a total of 4 bonds whereas B in BF₃ has only three bonds. Which matters more about the central atom:
the number of structural pairs or the total number of bonds
- III.3 Now consider the bond angles in Table III.2. In effect, the trend going from CH₄ to NH₃ to H₂O is to replace a bonded H atom with a lone pair. What effect does that have on the bond angles?

What is the reason for this trend?

PART IV-TORSION ANGLES

Lewis structure and torsion to measure	Value of Torsion Angle	Describe the relative positions of the outermost atoms
		
		
		

Part IV Questions:

IV.1 In the structure for CH_3CH_3 , are the H atoms on adjacent C atoms eclipsed (aligned) or staggered?

Which factor controls this, steric hindrance or bonding?

IV.2 Are the H atoms in the CH_2CH_2 eclipsed or staggered? Explain why.

IV.3 Describe the relative positions of the two Cl atoms in the third structure.

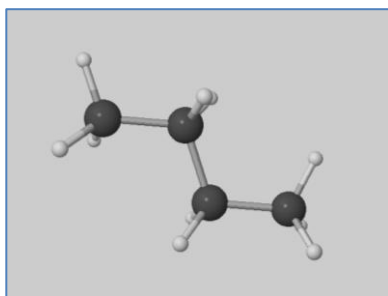
View the animation of your coordinate scan for $\text{CH}_2\text{ClCH}_2\text{Cl}$. To do this, select the coordinate scan in the Job Manager window. Next, select preferences (☰) and set the atom size to 100%. This will give a more accurate picture of the space taken up by each atom. Scroll down to the coordinate scan table. At the bottom of the table, select "Loop" in the looping options. Click on the animate icon (🎬) at the top of the coordinate scan table to view the movie of your results (you can rotate the molecule while the movie is playing).

Is the position of the two Cl atoms due to steric hindrance or bonding?
Explain your answer.

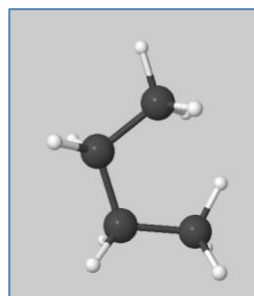
Scroll down to the coordinate scan table again and examine the energy associated with each conformation of $\text{CH}_2\text{ClCH}_2\text{Cl}$. To see a plot of energy vs. angle, you may also click on the view icon (🔍). The preferred angle is the one measured at the beginning of this exercise. What is the energy associated with this angle?

What is the energy of the conformation in which the Cl atoms collide?

IV.4 Predict which of the following conformations will be preferred for butane, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$. Circle the more stable (favored) conformation.



Conformation 1



Conformation 2

Which conformation will have a lower (more negative) energy?

PART V- PARTIAL CHARGES AND MOLECULAR DIPOLES

Table V.1- Partial Charges and Dipole Moments

		water H ₂ O	methane CH ₄	methanol CH ₃ OH	trifluoro- methanol CF ₃ OH	carbon dioxide CO ₂
Lewis Structure						
Partial Charge	H					
	O					
	C					
Formal Charge	H					
	O					
	C					
Oxidation Number	H					
	O					
	C					
Dipole Moment	Magnitude					
	Direction					

Part V Questions:

- V.1 Formal charge and oxidation numbers are the two main crude methods chemists use for counting electrons on atoms inside molecules. Partial charges are the reality. Consider the data in the table above. Which method more correctly represents the true distribution of electrons in molecules?
- V.2 Explain why the partial charge on H is different for CH_3OH and CF_3OH .
- V.3 Which compound would you expect to have stronger intermolecular hydrogen bonds, CH_3OH or CF_3OH ?
- V.4 Which compound would you expect to have stronger intermolecular hydrogen bonds, acetic acid ($\text{CH}_3\text{CO}_2\text{H}$) or trifluoroacetic acid ($\text{CF}_3\text{CO}_2\text{H}$)?
- V.5 What is the formula for the molecule you chose to build?
- V.6 Record the partial charges, formal charges, and oxidation number for each atom in your molecule.
- V.7 Does your molecule have a significant dipole moment? What is the magnitude and direction?

PART VI- MOLECULAR VIBRATIONS

Table VI.1- Vibrations in water and carbon dioxide

	Vibrational Frequencies (cm^{-1})			
	Symmetric Stretch	Asymmetric Stretch	Bending	
			Mode A	Mode B
water				X
carbon dioxide				

Carbon dioxide has two bending modes. Describe the difference in the type of motion for Mode A and Mode B:

Table VI.2- Number of atoms vs. number of vibrational modes

Compound	# of Atoms	# of Vibrational Modes
CH_4		
C_2H_2		
C_2H_4		
C_2H_6		

Based on your results above, predict which of the following molecules would have the most vibrational modes?

- | | |
|---------------------------|------------------------------|
| a. C_3H_8 | d. C_4H_{10} |
| b. C_3H_6 | e. C_4H_4 |
| c. C_3H_4 | |

Which of the following molecules would have the fewest vibrational modes?

- | | |
|---------------------------|------------------------------|
| a. C_3H_8 | d. C_4H_{10} |
| b. C_3H_6 | e. C_4H_4 |
| c. C_3H_4 | |