



## Worksheet: Vibrational Frequencies of Water

Name: \_\_\_\_\_

Date: \_\_\_\_\_

Class/Teacher: \_\_\_\_\_

### Instructions

Use this worksheet for your analysis of the data from the water frequencies log file (that you ran or that came from the uploaded log file). Follow the instructions from your teacher for submitting your work.

### 0.1 Basic Data Analysis

Open your job in the WebMO Job Manager, following the instructions in the lab. Answer these questions based on the output in the WebMO window

1. Rotate your molecule to get a sense of its shape. Click on the top curved arrow on the left-hand control panel to select rotate, then use your mouse to rotate the molecule. Describe the shape of this molecule. Look at it from top-down and from a side view:  
\_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

2. Click on the straight arrow in the left-hand control panel, then click on one hydrogen and the oxygen. Find the bond length (in units of angstroms, or Å) at the bottom left. What is your bond length? \_\_\_\_\_Å
3. Click on the second hydrogen, and find your bond angle in degrees at the bottom left. What is your bond angle? \_\_\_\_\_degrees
4. Most textbooks describe the bond angle of water at a value of 104.5°. Using the formula for percent error, where the calculated value is your measurement and the theoretical value is 104.5°, how accurate is the angle calculated by the computational chemistry server? \_\_\_\_\_% error

$$\text{PercentError} = \frac{|\text{Calculated} - \text{theoretical}|}{\text{theoretical}} \times 100 \quad (1)$$

5. In general chemistry, you should have learned the units of kcal/mole or kJ/mole as units of energy. Computational chemists use the energy unit of **hartrees**. Using the conversion factors of 1 hartree = 2625.5 kJ/mol = 627.5 kcal/mol, what is the energy (B3LYP Energy) of the water molecule?  
\_\_\_\_\_hartree = \_\_\_\_\_kJ/mol = \_\_\_\_\_kcal/mol
6. Water is a **polar** molecule. Imagine, if you will, a pole going through the oxygen atom. You can actually see this by going to "Calculate ->



Symmetry” option in the menu bar, then choosing ”C2”. If a molecule is polar, then there are a lot of electrons at one end of the pole (electron-rich, or negative end) and not many electrons at the other end (electron-poor, or positive end). Because the pole has two ends, we call it a **dipole**, and the measure of differences between the electron-rich end and the electron-poor end is called a **dipole moment**. This is a **vector**, a quantity that has both a *magnitude* and a *direction*. WebMO shows dipole moments with an arrowhead and plus vector line – the arrowhead is the electron-rich end, and the plus end is the electron-poor end.

- (a) Click on the magnifying glass next to the label ”Dipole Moment”. What is the magnitude of the dipole moment? Units are called *debyes*: \_\_\_\_\_debyes
- (b) What is the direction of the dipole moment? Where is the electron-rich end, and where is the electron-poor end? Describe why you think this is the case.

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7. You have learned in general chemistry that atoms have charges, mostly based on their position on the Periodic Table. In computational chemistry, we calculate what are known as **partial charges** on atoms, which represent some fraction of an electron. Using Table ?? below, list the charges for oxygen and hydrogen based on the Periodic Table, and then the partial charges from the quantum mechanics calculations:

Table 1: Charges on atoms

Atom	Charge from Periodic Table	Partial Charge
O		
H		
H		

8. Add up the charges from the Periodic Table column and from the Partial Charges column. What is the total charge on the water molecule?  
Periodic Table total charge: \_\_\_\_\_  
Partial Charges total charge: \_\_\_\_\_

## 0.2 Vibrational Frequency Analysis

Now we get to the heart of this lab, the analysis of vibrational frequencies.

1. Based on your understanding of the  $3N-6$  rule (where  $N$  is the number of atoms, how many vibrations do you predict for a water molecule?  
\_\_\_\_\_vibrations



2. Using Table ?? below, find your vibrational frequencies from the WebMO Job Manager. Using your percent error formula, compare your results (calculated) with the experimental values. Also, using the chart showing the different types of vibrations (stretching, rocking, scissoring, etc.), determine what kind of vibration each one represents. If you click on the icon that looks like a movie icon next to each vibration, you can see an animation of the vibration!

Table 2: Data table for vibrational frequencies

Mode	Experimental Value ( $\text{cm}^{-1}$ )	Calculated Value ( $\text{cm}^{-1}$ )	Percent Error	Type of vibration
1	1713.1018			
2	3727.3599			
3	3849.3997			