



## Worksheet: Vibrational Frequencies of Ethylene (Ethene)

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

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

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

### Instructions

Use this worksheet for your analysis of the data from the ethylene 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 Data Analysis

Open your job in the WebMO Job Manager.

1. How many atoms are in ethylene? \_\_\_\_\_
2. Using the  $3N-6$  rule, where  $N$  is the number of atoms, how many vibrations do you predict? \_\_\_\_\_
3. From the output window, locate the panel entitled "Vibrational Models". How many vibrations have been identified? \_\_\_\_\_
4. Look at Figure 1. This chart shows all 12 vibrations. The arrows indicate the motion of various atoms in the molecule. The plus signs signify atoms coming *out* of the plane of the paper, towards you. The minus signs signify atoms going *into* the plane of the paper, away from you. These motions are, of course, relative depending on how you have your molecule oriented.

In the WebMO vibration panel, you should see the frequencies listed as wavenumbers ( $\text{cm}^{-1}$ ). You should enter those values as data in Table 1 below. Note that the values in this table and in your output window will not necessarily be in the same order, so you should enter your results data matching the closest frequency pairs.

You have two options for viewing the frequencies. If you click on the magnifying glass, you get a static representation with arrows showing motion. Clicking on the movie strip icon shows you an animation, and this is the recommended procedure. In your data table, you want to be able to describe the type of vibration represented by a specific frequency – rocking, wagging, scissoring, etc.

Use one, or both, of the representations to decide which representation in Figure 1 corresponds to which vibration in your output window.

5. You might want to do a percent error estimate comparing computed and experimental frequencies. Use your experimental frequencies as the theoretical quantity in the equation below:



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

6. Complete the table. For the column labeled "Number of vibration", you want to enter the number (1 through 12) corresponding to Figure 1.
7. Optionally, you might want to perform a linear regression ( $y=mx+b$ ) analysis of your experimental and calculated data. Use the computed data as the independent value  $x$  and the experimental frequencies as the dependent variable  $y$ . It is known that the computed results are off by a small amount, so we use a scaling factor of about 96% (0.96) to scale experimental values to computed values. The slope of your line is the scaling factor. What scaling factor do you get for you data? \_\_\_\_\_

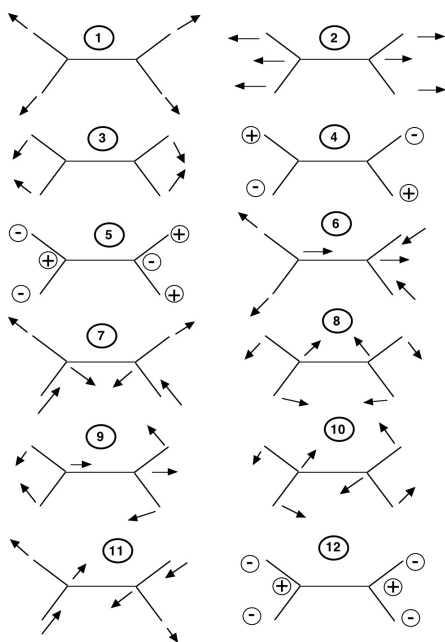


Figure 1: Ethylene vibrations chart. The ID numbers assigned to each vibration are arbitrary, and do not correspond to the modes seen in the results window



Table 1: Data Table for Ethylene Vibrations

Mode	Experimental Frequency (cm-1)	Computed Frequency (cm-1)	Number of Vibration from graphic of ethylene vibrations	Type of Vibration	Percent Error
1	845				
2	957				
3	965				
4	1043				
5	1241				
6	1378				
7	1482				
8	1650				
9	3036				
10	3051				
11	3099				
12	3130				