

CH 114 Principles of Chemistry II
Spring 2001
Computer Project II - Analysis of Nuclear Magnetic Resonance Data

(200 points + 20 points extra credit)

Names (print) _____

*This is a group project (two people) and only one report will be turned in for the entire group; however, it is important that each individual contribute substantially and equitably to this project. Complete the following project, applying the graphing and computer skills learned in the Principles of Chemistry courses. Submit a report, constructed with either Word or WordPerfect word processor, with a coversheet that clearly indicates an appropriate title, the date submitted and the co-authors of this report. **This handout and attached data must immediately follow the coversheet.** The body of the report should be broken down into sections which answer each of the problems noted below. Be sure to clearly show your answer for each problem, and give a concise rationale for your answer. At the end of the report, each student should write a paragraph describing what they contributed to this project and then sign below that paragraph. Each of their partners should then initial below this signature if they agree with their partner's assessment. This assignment is to be turned in at check-out time.*

Introduction

In this computer project you will be required to analyze large amounts of data with Excel or SigmaPlot. Normally, the tasks you will be performing are carried out fast, seamlessly, and behind-the-scenes by a computer program that is specifically designed for the task. However, it is many times important to understand how these different operations are done by carrying them out by hand.

The data that you will be analyzing comes from the same nuclear magnetic resonance (NMR) experiment that you will perform in the last laboratory of the semester. It represents an NMR spectrum of the hydrogen atoms in a molecule called **sodium borohydride (NaBH₄)**. At this point, knowledge of what the spectrum looks like or represents is not entirely required, but it may be convenient for you to download and read the handout that corresponds to the NMR experiment (**week12.pdf**).

- 1) (20 points) Go to the Principles of Chemistry 114 web page and download a copy of the data set for computer project II (**comp11.txt**). Make sure that you save it as a **text file** when you download it, and remember to save it to your floppy diskette.
- 2) (40 points) Once the data is securely saved in your diskette, open it with Excel or SigmaPlot. You may have to help the program understand what type of data you are

reading in. It should be in **text** file format. At this point you should have a new data sheet with a single column.

Create an additional column that has the number of rows present in the data column. Now plot the data (or spectrum), using the column with row numbers as your **x** axis and the data column as your **y** axis. You should see one large peak to the left, and a complicated pattern on the right with four tall peaks and seven short peaks.

The spectrum that you are plotting is a function of frequency which has units of **Hertz (Hz)**, and the separation between data points in the x axis is 0.3662 Hz. Create a new column with the frequency, starting at a frequency of 0.0 Hz (Hint, the frequency increment for each cell of the new row should be 0.3662 Hz). Now create a new plot in which you have frequency in the **x** axis and the data in the **y** axis.

Finally, create a new column in which the data is **normalized** (i.e., its maximum value is 1). For this you will need to find the maximum value of the data, and divide all data points in the data column by this number. Again, once you are done with this plot the normalized data column against the frequency column.

- 3) (40 points) Now you will calculate the derivative of the normalized spectrum. For this, create a new column whose cells are $\Delta y/\Delta x$. Remember, Δy is $(y_i - y_{i-1})$, and Δx is $(x_i - x_{i-1})$.

Once you have created a new column with the derivative of the spectrum, plot it against the frequency.

As you did in part (2), normalize the derivative, but beware: The value with the maximum magnitude could be negative, in which case you will have to normalize the data using its absolute value.

Once you normalized the derivative, plot the spectrum and its derivative in a single graph.

- 4) (40 points) Now that you computed derivatives, you will calculate the integrals of the spectrum. For doing so, you will have to create a new column in which each cell is equal to the sum of all the cells preceding it. That is, if you want to calculate the integral at point i , I_i , it will be $I_i = V_i + V_{i-1} + V_{i-2} + \dots + V_0$, where V_i is the value of the normalized spectrum that you calculated in part (2).

As you did for the derivatives, once you created the new column with the integral of the spectrum plot it against the frequency.

- 5) (60 points) As it was mentioned above, the relevant region of the spectrum is the one showing the complex set of 11 signals. As you will learn in the NMR experiment, the larger 4 are related to boron 11 (^{11}B), and the 7 shorter ones to boron 10 (^{10}B). Thus, if you calculate the ratios between the summed areas below the large peaks

to the summed areas under the shorter peaks, you can get a good estimate of the $^{10}\text{B}/^{11}\text{B}$ isotopic ratio in Nature. To do this, you will have to perform the following operations: First, calculate the individual areas (i.e., the integrals) of the 4 large peaks, and then for the 7 small peaks. To calculate them you have to repeat the procedure done in part (4), but not for the whole spectrum - The integrals need to be calculated only for the frequency region corresponding to each peak. These are:

Tall peaks:	1) 460-480	Short peaks:	1) 500-515
	2) 540-555		2) 530-540
	3) 620-635		3) 555-570
	4) 700-720		4) 580-600
			5) 605-620
			6) 635-650
			7) 660-680

Once you calculate all the individual areas, add the ones corresponding to the tall peaks (^{11}B), and also those corresponding to the shorter peaks (^{10}B), and record both numbers. Calculate the ratio between these two numbers as a percentage, and compare this to the reported value for the $^{10}\text{B}/^{11}\text{B}$ isotopic ratio. In your report, present a table with the values of all the individual areas, the summed areas, and the calculated $^{10}\text{B}/^{11}\text{B}$ isotopic ratio.

Good luck!