Experiment 2

SPREADSHEETS AND CHARTS

**Exercise 1 and 3 should be handed in as a soft copy.**
**Exercise 2 and 4 should be handed in as a hard copy.**

Please bring a USB (“flash”) drive on which to store your work.

Exercise 1

Create the EXCEL spreadsheet and chart described in section 2-10 of the Harris textbook.

Create an exact replica of the chart shown in Figure 2.20 (data and graph) following the directions given in Sections 2-10 and 2-11. Save the file on your USB drive and email it to me. Label the sheet in your file you send as Exercise 1.

Exercise 2

Using the Excel spreadsheet and chart, find the density of water at 35 °C and at 20 °C.

If you dissolve 1.0000 g of Na₂CO₃ in a 250.0-mL volumetric flask and dilute to volume with water at 35 °C, calculate the molarity of this solution at 20 °C. (Hint: You have enough data to directly calculate the molarity at 35 °C. However, the volumetric flask is calibrated for solutions at 20 °C. Therefore, the solution volume at 20 °C will be different than the one at 35 °C (which is 250.0-mL). This “corrected” volume can be calculated using the graph that shows a plot of density vs. temperature, so the molarity at 20 °C can readily be calculated.)

Calculate the % relative error in the molarity of the solution which you just prepared using the following equation:

\[
% \text{ error} = \left( \frac{\text{Molarity at } 35 \degree \text{C} - \text{Molarity at } 20 \degree \text{C}}{\text{Molarity at } 20 \degree \text{C}} \right) \times 100 \quad [2.1]
\]

Pay attention to the sign (+ or −) for the % error.

Hand in all calculations associated with Exercise 2. Neatly hand-write these calculations and title Exercise 2.

Exercise 3

Create an Excel spreadsheet that displays the following data.
<table>
<thead>
<tr>
<th>Fe concentration (ppm)</th>
<th>Absorbance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>-0.001</td>
</tr>
<tr>
<td>0.5</td>
<td>0.051</td>
</tr>
<tr>
<td>1.0</td>
<td>0.102</td>
</tr>
<tr>
<td>2.0</td>
<td>0.199</td>
</tr>
<tr>
<td>4.0</td>
<td>0.411</td>
</tr>
<tr>
<td>8.0</td>
<td>0.829</td>
</tr>
</tbody>
</table>

To adjust the number of decimal places, select the corresponding cells, click on “Format”, select “Cells”, then select “Number” and insert the number of decimal places for the column (1 for concentration, 3 for absorbance).

Generate a third column that shows absorbance corrected for the absorption of the blank. (Corrected absorbance is obtained by subtracting the blank absorbance from each individual absorbance value. The absorbance of the blank is the value for a concentration that is equal to 0.)

Create a plot that displays a dependency of corrected absorbance on concentration (select the “XY scatter” option with visible data points for the graph). Click “Next” and then select the “Series” menu. Click in the box for X value and then select all the X-values (concentration) on the spreadsheet. Click “Enter”. Then click in the box for Y value and select all the Y values (corrected absorbance) on the spreadsheet that you want displayed. Click “Enter”. Name the graph and label the axes (units too).

To perform a linear regression in an EXCEL spreadsheet, move to the Tools menu and select Data Analysis. Select Regression. Click in the Y-range box, then move to the spreadsheet and select the Y-range data (the absorbance data in this example). Then click in the X-range box and then select the X-range data. Now click the Output Range button. Click in the associated box, then move to the spreadsheet and click in a cell where you would like the regression output to begin. The regression output will fill up space to the right and down from this box, so choose a cell that is below your experimental data. Now click the OK button of the Regression Box. EXCEL will perform the regression calculation and place the output on your spreadsheet. Scroll down to find the table that contains information on the intercept and X-Variable (slope). The “Coefficient” Column is the value of each of these linear parameters and the “Standard Error” column is a measure of the uncertainty or standard deviation in each.

Annotate the chart with the regression equation and the standard deviation (often called standard error in a spreadsheet) for the slope, $s_m$ and y-intercept, $s_b$, of the regression line. Save a copy of your spreadsheet and chart on your flash drive. Print out the spreadsheet containing the graph and the regression analysis.

There are two ways to place the regression line on your chart showing the experimental data. The first is to create an additional series to plot, using the regression equation to calculate a Y-value for each X-value. You would want to format this series so that a line was plotted without any symbols showing. A simpler way to show the regression line is by using the trend line function on the chart menu. Note, however, that
the trend line function of the Chart menu does not give the uncertainty of the slope and intercept, therefore you must perform a linear regression analysis of the data, in the spreadsheet, even if you use the trend line function to display the line on the chart.

Email this to me along with Exercise 1 as a separate sheet labeled Exercise 3.

Exercise 4

a) Using the regression line equation, calculate the iron concentration (in ppm) if an unknown gives an absorbance of $A_{\text{unknown}} = 0.150$.

To calculate the iron concentration, note a general equation for a straight line:

$$y = mx + b$$  

where $y$ is the dependent variable (in our case, corrected absorbance, $A$), $x$ is the independent variable (in our case, iron concentration, $[\text{Fe}]$), and $m$ and $b$ are the slope and the intercept of the line, respectively.

Thus, the equation above can be rewritten as:

$$A = m[\text{Fe}] + b$$  

This relationship, obtained by plotting the corrected absorbance of solutions with known iron concentrations, is a calibration line for the analysis. The mathematical expression for this line is given by the regression line displayed in your graph.

Further, Eq. [2.3] is solved to obtain the iron concentration of the unknown solution.

$$(A_{\text{unknown}} - b)/m = [\text{Fe}]_{\text{unknown}}$$  

b) Calculate the uncertainty in the iron concentration at a 95% confidence interval following the procedure described below.

As with any measurement, there is uncertainty associated with it and it must be estimated. There is uncertainty in the absorbance, $A$, the slope, $m$, and the intercept, $b$. Eq. [2.4] can be rewritten as follows:

$$\{(A \pm s_A) - (b \pm s_b)\}/(m \pm s_m) = [\text{Fe}]$$  

In order to estimate the uncertainty in the iron concentration, first propagate the absolute uncertainties in the numerator to find the uncertainty in that value. Then propagate the relative uncertainties in the numerator and denominator to get the relative uncertainty in the iron concentration. Then calculate the absolute uncertainty in the iron concentration. (Alternatively, use equation 4-27 from the text)

Finding the uncertainty in the slope and intercept was discussed above. The uncertainty in the absorbance is found as the standard error under the heading of “Regression Statistics” near the top of the Summary Output.
c) To calculate a 95% confidence interval from the standard deviation, use the confidence interval equation with n–2 degrees of freedom, where n is the number of data points on the calibration line.

Neatly hand-write these calculations and label Exercise 4 to hand in.