Determining the Activation Energy of a Chemical Reaction

In lab this week you will measure the activation energy of the rate-limiting step in the acid catalyzed reaction of acetone with iodine by measuring the reaction rate at different temperatures. Rate data as a function of temperature, fit to the Arrhenius equation, will yield an estimate of the activation energy.

$$\ln k(T) = \frac{-E_a}{R}\left(\frac{1}{T}\right) + \ln A \qquad\qquad \ln k(T_2) - \ln k(T_1) = \frac{-E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

slope-intercept form   point-slope form

From the Arrhenius equation, a plot of ln(k) vs. 1/T will have a slope (m) equal to $-E_a/R$. R in this case should match the units of activation energy, R= 8.314 J/(K mol). In lab you will record the reaction rate at four different temperatures to determine the activation energy of the rate-determining step for the reaction run last week.

To determine the activation energy of the rate-determining step you will run the iodine acetone reaction at room temperature and at 45 °C, 35 °C and 15 °C. From the iodine acetone reaction you ran last week, select a set of reactant concentrations that ran successfully. This set of reagent concentrations will be used throughout the temperature study.

Experimental Procedure:

- Obtain 100 mL of 4.0 M acetone, 100 mL of 1.0 M HCl and 50 mL of I_2 solution in beakers. Keep a watch glass over the reagent beakers while not in use.

Keeping a reaction at a fixed temperature takes some experimental care. It is no good to have a flask in a water bath at 40 °C and then place reagents that are at 22 °C in the flask and expect to know the temperature.

- In a 1000 mL beaker (obtained from the front of the room) prepare a water bath at room temperature.

- Clamp your 125 mL Erlenmeyer flask into the water bath along with a thermometer and a test tube to hold your I_2 solution. A schematic for this set-up is given on the next page.

- Measure and pour the amounts of acetone and HCl that you will use in the reaction into the 125 mL reaction flask. Pour into a clean test tube the amount of I_2 to be used in the reaction. Clamp each solution into the water bath and let it sit for five minutes to equilibrate to the bath temperature.

- After the 5 minutes of equilibration, record the water bath temperature. This will be the reaction temperature. Remove the I_2 solution from the clamp and quickly add it to the reaction mixture. At the same time you add the I_2 solution, begin timing the reaction. Swirl the reaction mixture initially by swirling the whole ring
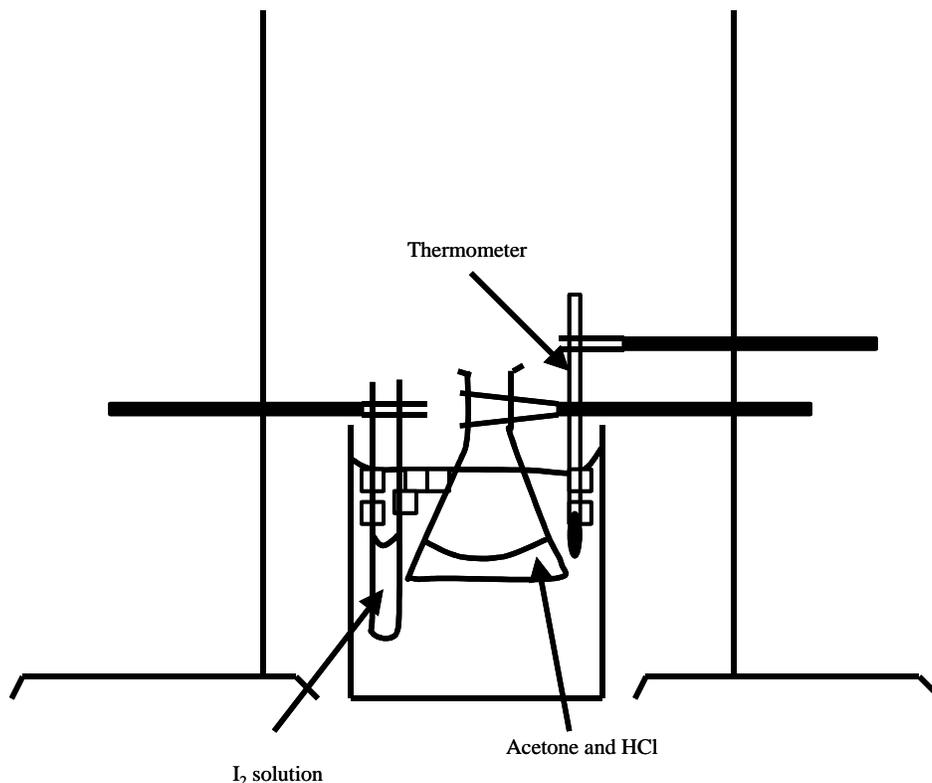
stand. After an initial shake the reaction can be left to sit. When the iodine color is gone the reaction is complete.

Figure 1: Schematic of the water bath used in the temperature rate study. Allow the reactants to equilibrate in the bath temperature for 5 minutes.

- When the reaction is completed, clean your glassware and prepare to run the reaction in a new water bath. The I_2 test tube does not need to be cleaned since it will always contain the same concentration of liquid.

- From the reaction time and the initial I_2 concentration, determine the reaction rate at this temperature.

- Using warm water from the sink, run the reaction at a temperature between 30 and 38 °C. In a third set of experiments run the reaction in a water bath that is between 40 and 45 °C. In each case the specific temperature of the reaction is not important, as long as you record what the temperature is **exactly**. For a low temperature run, prepare an ice bath that is between 10 and 15 °C. If you prepare a 0 °C ice bath you will be in lab well after 5:30 waiting for the I_2 to react.

- After determining the reaction rate at four different temperatures between 10 – 50 °C, clean your glassware and return your 1000 mL beaker, thermometer and ringstand to the front of the room.

Data Analysis:

To determine the activation energy, create an Arrhenius plot of the rate vs. temperature data. Recall that a linear relationship exists for ln(rate) vs. 1/T(K). The plotting can be done using Microsoft Excel.

Plotting in Excel:

There are many plotting programs that are easier to use and that make better presentations of scientific data, but no program is more popular than Microsoft Excel, so it won't hurt to learn a little about it.

In the computer lab open Excel. Below is a figure of how the spreadsheet should appear before plotting. Begin by labeling column A, Temp(C)

Figure 2, Screen capture of the Excel spreadsheet showing the data input for making an Arrhenius plot.

Enter the Temperature data using units of °C in Column A. You need only enter the Temperature and Rate data. The formula feature in Excel will calculate 1/T and ln(rate) for you.

Label column B, Temp(K). In the cell B2 enter the formula "=A2+273.15". The equal sign tells Excel that you want to do a calculation. Click the check button when the formula has been entered.
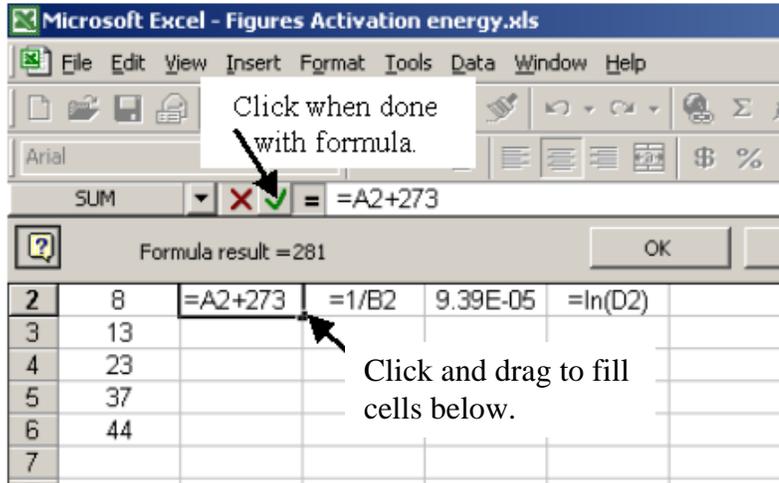

Figure 3, Excel spreadsheet focusing on the method for entering a cell formula.

After the formula is entered it can be copied to the other cells below it by clicking on the black box in the bottom right corner and dragging to the cells below.

Refer to Figure 2 to complete the rest of the data entry and calculations using these Excel techniques.

To plot the data, click and drag over the 1/T column to highlight the column and then with the Ctrl button pressed drag on the ln(rate) column. Each column should be highlighted as in Figure 2.

To plot this data click on the Chart Wizard Icon, .
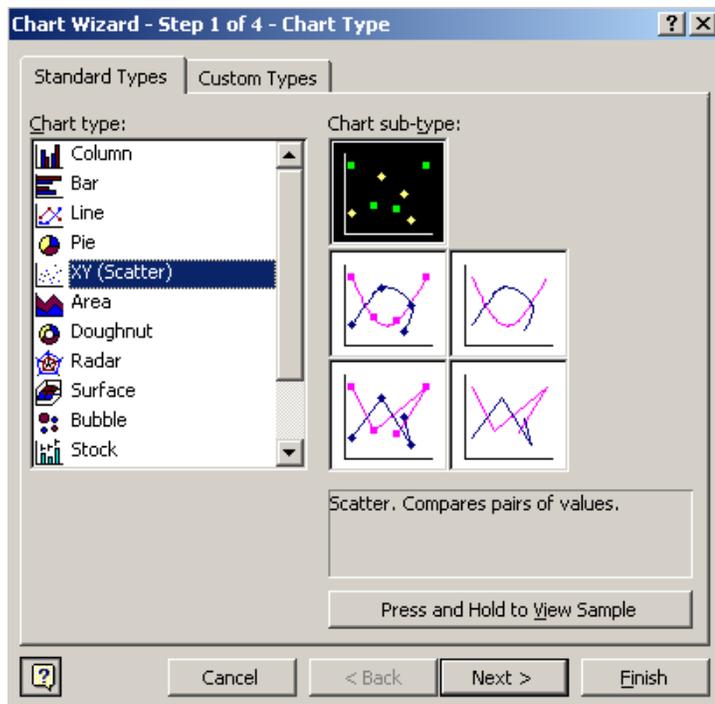
Figure 4, Screen capture of the Excel spreadsheet showing the Chart Wizard dialogue box. Select XY (Scatter), no points connected.

In the Chart Wizard select XY (Scatter) and points only. Then click Finish. The resulting plot should look similar to the following.
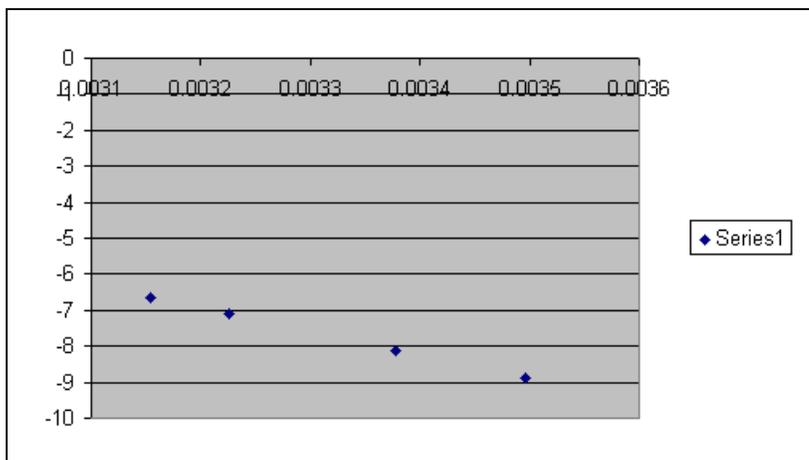
Figure 5. View of the default data plot from Excel.

Quite frankly this is an ugly plot and should be edited to something that looks more like the plot in Figure 6.
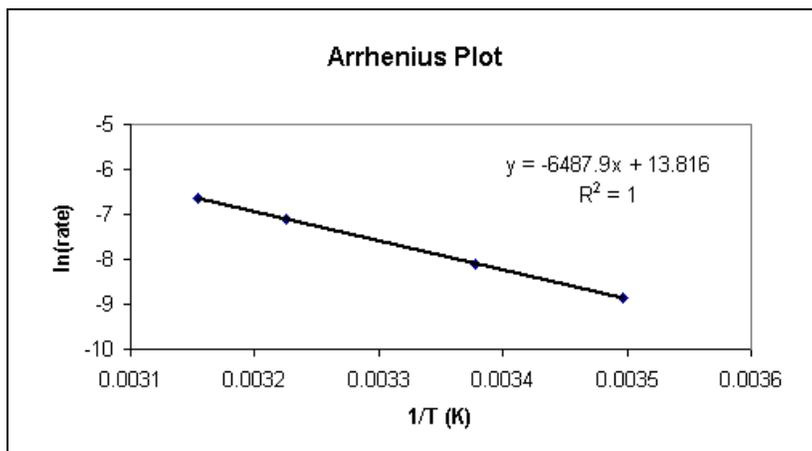
Figure 6. View of the Arrhenius plot after editing.

The cleaning up of the plot takes some editing. Talk to someone in the computer lab or your instructor to make the appearance changes to the plot. This will be a figure in your lab report, so it is worth making it look nice.

The linear fit to the data is done in Excel by right clicking on a data point and selecting "Add Trendline". In the trendline dialog box select the type as "Linear" and then click on the options tab. In the options box, click the "Display Equation on Chart" feature. The best-fit line will be given to you in slope-intercept form. Expect a slope similar to the slope given in Figure 6. Save this Plot to your network drive. You will want to include this figure in the Discussion section of your lab report.

From the slope determine the activation energy of the reaction, reported in kJ/mol.