Name____________
Class_____________
Date_____________

EXPLORING THE TEMPERATURE DEPENDENCE OF THE EQUILIBRIUM CONSTANT (K) WITH THE TI-NSPIRE

Discussion:

The equilibrium constant (K) for any given reaction does not vary as long as the temperature of the reaction remains constant. The usual temperature for equilibrium calculations is room temperature (25°C). If the temperature varies from this standard, then the equilibrium will shift left or right depending on whether the reaction is endothermic or exothermic and the value of K will either increase or decrease accordingly.

The relationship between equilibrium (K) and Celsius temperature is not a linear relationship. To obtain a linear relationship, the reciprocal of the Kelvin temperature must be plotted against the natural log (Ln) of K. When graphed in that fashion the linear regression equation will take the form:

$$\text{Ln K} = -\left(\frac{\Delta H^0}{R}\right)\left(\frac{1}{T}\right)+\left(\frac{\Delta S^0}{R}\right)$$

where the slope of the line is $-\left(\frac{\Delta H^0}{R}\right)$ and the y-intercept is $\left(\frac{\Delta S^0}{R}\right)$. The thermodynamic value of R is 8.3145 J/Kmol.

Objective:

In this activity the student will use the List and Spreadsheet, Graphs and Geometry, and Calculator applications to analyze the relationship between temperature and the equilibrium constant (K). The student will use the following functions:

1. enter data into lists
2. name lists
3. use formulas to populate data
4. determine regression equations
5. graph data
6. plot regression lines
7. use the calculator application

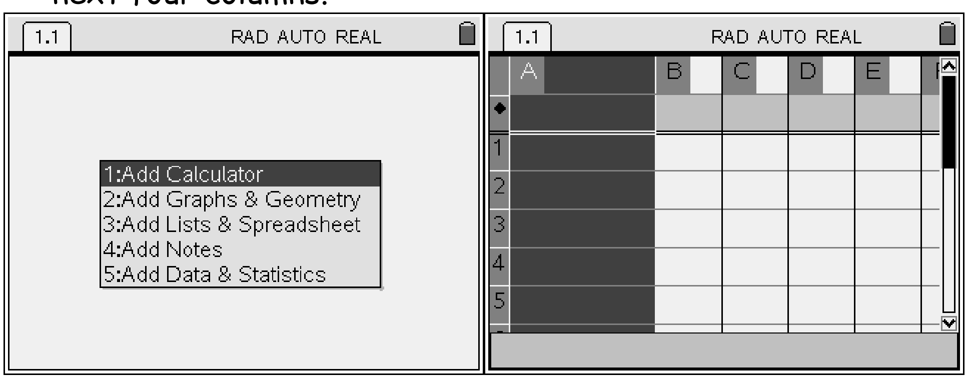
Procedure:

A. The equilibrium reaction that we will be working with is:

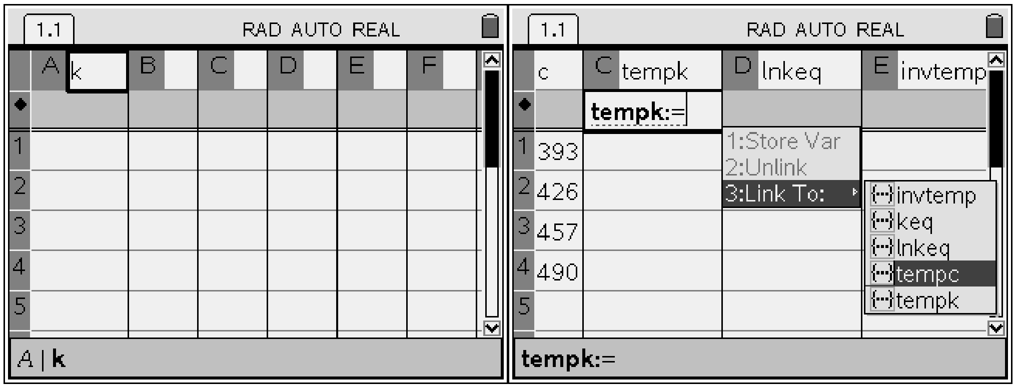
$$2HI_{(g)} \rightleftharpoons H_{2(g)} + I_{2(g)}$$

B. As we prepare to begin this experiment, let's consider the following questions:
   1. What effect does an increase in temperature have on the value of K?
   2. Is this an endothermic reaction or an exothermic reaction? Justify your answer.
   3. If this reaction were to be used to produce iodine, how could the temperature be changed to increase that yield?

C. Turn on the TI-Nspire and choose the on the upper right. Choose New Document. If asked to save a document, choose No. Choose Lists and Spreadsheets. When the spreadsheet opens, choose the on the upper right, choose Actions and choose Resize. Press the on the NavPad twice to make the first column wider. When the column is the desired width, press and then . Repeat for the next four columns.



D. Move the cursor into the heading space of Column A and type in K as the List name and press . Type in tempC as the List name for Column B. Press . Type in tempK as the List name for Column C and press . Type in LnK as the List name for Column D and press . Type in invtemp as the List name for Column E and press .



E. In Column A, enter the K reading from the table below. In Column B, enter the Celsius temperature readings.

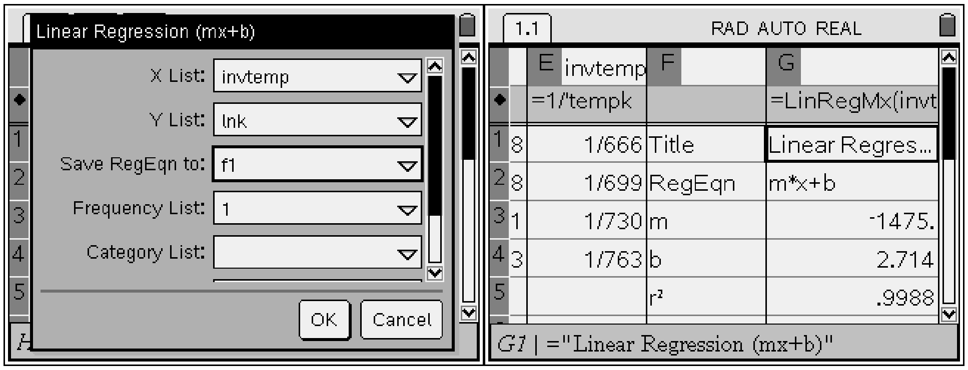
K	T(^{0}C)	T(K)	Ln(K_{eq})	1/T(1/K)
1.65	393			
1.82	426			
2.01	457			
2.18	490			

F. To complete Column C (tempK), it is necessary to create a formula in Column C that adds 273 degrees to the Celsius temperature in Column B. Move the cursor to the formula cell (**in gray**) in Column C and press (=). Then press the (sto▸ var) key and Link to the tempC variable and press (enter). Press the (+) and 273. Press (enter) to populate the column. Copy the calculated data into the table above.

G. To complete Column D (lnK), move the cursor to the formula cell in Column D and press =. Then choose Ln by pressing the (ctrl) and (ln e^x) keys. Press the (sto▸ var) key and Link to K. Press (enter) to populate the column. Copy the calculated data into the data table above.

H. To complete Column E (invtemp), move the cursor to the formula cell in Column E and press (=). Then press 1, the (÷) key, and press (sto▸ var) and Link to, and choose tempK. Press (enter) to populate the column. Copy the calculated data into the data table above.

I. We can analyze the relationship between Ln K and 1/T to determine if it is, in fact, linear by calculating the regression data.



J. To perform a regression, select Stat Calculations from the Statistics menu. Since the relationship between LnK and 1/T should be linear, we choose to perform a Linear Regression (y = mx + b). For the X-list, press the NavPad ▼ and choose invtemp by pressing enter. tab down to the Y-list and use the NavPad ▼ key to choose LnK by pressing enter. tab further to 1st Result Column, choose the letter F, and press enter to populate Columns F and G with the Linear Regression Data. Record the Regression data with appropriate **units** below:

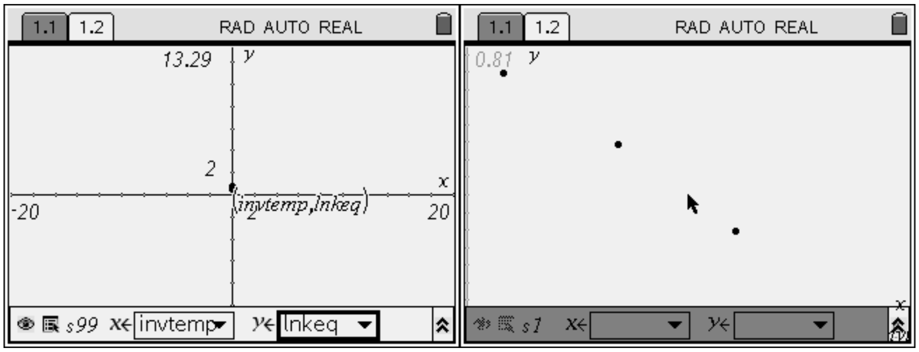
m=____________

b=_____________

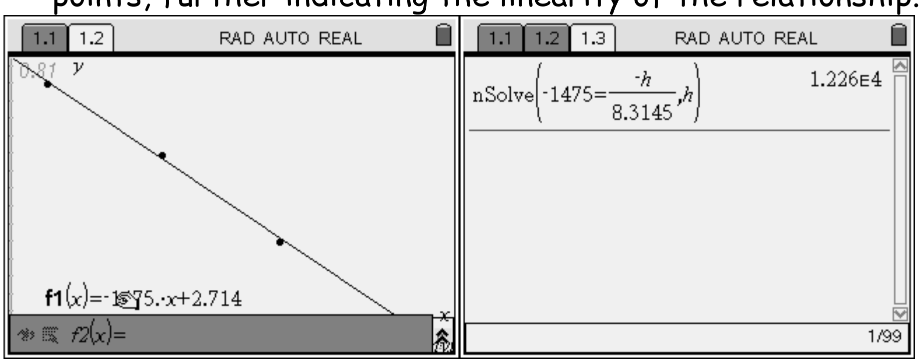
r=_____________

K. The correlation coefficient (r) for the data is nearly an absolute value of 1, so the data appears to be linear. To graph the data with the regression function, in the Graphs and Geometry application. Press the ctrl key and the letter I to insert a new Graphs and Geometry page.

L. Draw a scatter plot of Ln K and 1/T, choose Menu, Graph Type, Scatter Plot. Press enter to choose the x variable which is invtemp and press enter. Press Tab, then press enter to choose the Y-variable (select lnKeq). Adjust the window by pressing Menu, Window, Zoom-9. The scatterplot will be displayed. Make a sketch of the graph with axes labeled and proper units included in the space below.



M. To plot the regression equation, press Menu, Graph Type, and function. Press the ▲ on the NavPad to access f1(x), and press enter to draws its graph. The regression line passes through each of the points, further indicating the linearity of the relationship.



N. To calculate the ΔH^o **and** ΔS^o, it is necessary to use the Calculator application. Press the ctrl key and the letter Ⓘ to insert a new Calculator page.

O. To calculate ΔH^o, we need to set the slope equal to $-\left(\frac{\Delta H^0}{R}\right)$. The slope was determined to be -1475 K. The value of R is 8.3145 J/Kmol. Choose Menu, Calculations, Numerical Solve. Inside the parentheses, enter (-1475 = -h/8.3145, h) and press Enter. The value of ΔH^o will be given.

P. The y-intercept was determined to be 2.714. To calculate ΔS^o, repeat the process to insert Numerical Solve once again. Inside the parentheses, enter (2.714 = s/8.3145, s) and press Enter. The value of ΔS^o will be displayed.

Q. Record the value of ΔH^o and ΔS^o with the appropriate **units** below:

ΔH^o_______________

ΔS^o________________

R. The ion product of water is K_w. The ion product is the hydrogen ion $[H^+]$ concentration times the $[OH^-]$ concentration.

1. What effect does an increase in temperature have on the value of K_w?
2. Is this an endothermic reaction or an exothermic reaction? Justify your answer.

S. Repeat the process of calculating ΔH^o and ΔS^o for the following data:

K_w	$T(^0C)$	T(K)	$Ln(K_w)$	1/T(1/K)
1.14×10^{-15}	0			
1.00×10^{-14}	25			
2.09×10^{-14}	35			
2.92×10^{-14}	40			
5.47×10^{-14}	50			

T. What do you expect to happen to the data in the linked columns when this new data is entered? Why does this change occur?

U. Fill in the data table above with the appropriate data from the Lists and Spreadsheets application.

V. Make a sketch of the graph with axes labeled and proper units included. Record the regression statistics with **appropriate units** below:

m=____________

b=_____________

r=_____________

W. Calculate the value of ΔH^o and ΔS^o as before and record below with appropriate **units**:

ΔH^o_______________

ΔS^o________________

Extension:

1. From the K_w data above, calculate the pH of water at each of the temperatures given?
2. Does neutral water always have a pH of 7? Why or why not?
3. Why is it necessary to specify temperature when measuring or recording pH values?

Self-Evaluation:

You will be expected to master the skills taught in this exercise in order to complete homework problems. Final evaluation will be the use of those skills to solve similar problems on the Thermodynamics Unit Test. Evaluate your mastery of these skills for the second exercise for K_w.

Skill	**Complete activity without referring to instructions (3 points)**	**Complete activity with reference to instructions (2 points)**	**Complete activity with teacher assistance (1 point)**
Enter data into lists			
Name lists			
Use formulas to populate data			
Determine regression equations			
Graph data			
Plot regression equations			
Use the calculator application			