CH113
Principles of Chemistry I Laboratory
Fall 2000
Computer Project II
F

Names _____

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(240 pts + 20 pts extra credit)

print

This is a group project which will involve the use of computer programs to both model and analyze thermochemical data. You are to use SigmaPlot or Excel programs found on the computers in G-222C to construct all plots; You may use either SigmaPlot, QuattroPro or Excel spreadsheets to perform the calculations. You must turn in clearly labeled graphs and spreadsheet tables with your final report. You are to save all this information on a new 3.5" floppy disk. This disk should only be used on these computers.

This is a group project 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. Therefore, complete the following project applying the graphing and computer skills learned in the Principles Laboratory. Submit a report with a coversheet that clearly indicates an appropriate title, the date submitted and the coauthors of this report. The next two pages must include these two pages of this handout. The body of this 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. Show which equations that you used in your transforms. 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 **must** be turned in at the beginning of the lab period of the week of November 28th.

1. A student collected the following thermodynamic equilibrium constants for the reaction

$$A\,(g) + 2B\,(g) \leftrightarrow 2C\,(g)$$

at various temperatures.

T (^{o}C)	20.00	30.00	40.00	50.00	60.00	70.00	80.00	90.00
K	3.3×10^{-01}	6.5×10^{-01}	1.2×10^{00}	2.1×10^{00}	3.7×10^{00}	6.2×10^{00}	1.0×10^{01}	1.6×10^{01}

a) (40 pts) Use a spreadsheet to create columns which show the values for the absolute temperature, 1/absolute temperature, natural log of the equilibrium constants and ΔG^{o}(kJ) for this reaction at each of the indicated temperatures.

b) (30 pts) On separate graphs, plot K vs. T(K) (i.e. Y vs. X), ln K vs. T(K) and ln K vs 1/T (K^{-1}). Be sure to adjust the axes to cover an appropriate range, properly label each axis and give a proper title to each graph.

c) (30 pts) Use SigmaPlot to plot the best line through the plot of the graph of ln K vs. 1/T. Use the regression wizard of SigmaPlot to determine the slope and intercept and their associated errors of this plot.

d) (20 pts) Determine the values and the associated errors of ΔH^o(kJ) and ΔS^o(J/K) from the information in problem c. Indicate these values by typing them on the graph. (e.g. "ΔH^o = xxx.x ± y.y kJ")

e) (30 pts) The student performs a second experiment in which the initial partial pressures are: P_A = 0.500 atm; P_B = 0.250 atm; and P_C = 0.500 atm at each of the above temperatures. From this information, calculate the value of Q and ΔG(kJ) at each of the listed temperatures and plot ΔG^o and ΔG(kJ) vs. T(K) on the same graph. Be sure to adjust the axes to cover an appropriate range, properly label each axis, provide a suitable key and give a proper title to the graph.

f) (40 pts) At each temperature in 1e, describe whether the nonequilibrium reaction is: endo- or exothermic; becoming more or less ordered; must go toward products or reactants in order to come to equilibrium; and will be spontaneous or not spontaneous as written.

g) (60 pts) Determine the value of K, ΔH^o, ΔS^o, ΔG^o, Q, and ΔG for this reaction at 56.23°C under conditions where P_A = 0.623 atm, P_B = 0.324 atm, and P_C = 1.250 atm.