CH114
Principles of Chemistry Laboratory II
Spring 2001
Computer Project I

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 acid/base data. You are to use the SigmaPlot program found on the computers in G-222C to construct all plots; You may use SigmaPlot 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 three pages must include the first three 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 is to be turned in to Dr. Moyna at the beginning of your lab period on Tuesday, Februrary 6th.

1. An aqueous solution contains _______ M HCl(aq). 15.00 mL of this solution is titrated with a 0.173 M KOH(aq) solution at 25°C.

a) (30 pts) Construct a computer generated table that will show the following information as a function of the volume of added KOH solution from 0 to 20 mL in 0.5 mL increments (assume that the volumes are additive): V_{KOH}(mL), V_{total} (mL), $[H_3O^+]_{init}$, $[OH^-]_{init}$, $[K^+]_{eq}$, $[Cl^-]_{eq}$, moles $H_30^+_{eq}$, moles OH^-_{eq}, $[H_3O^+]_{eq}$, $[OH^-]_{eq}$, pH and pOH

b) (20 pts) Construct a graph which contains plots of $[K^+]_{eq}$, $[Cl^-]_{eq}$, $[H_3O^+]_{eq}$ and $[OH^-]_{eq}$ as a function of V_{KOH}(mL).

c) (10 pts) Construct a graph which contains plots of moles $H_30^+_{eq}$ and moles OH^-_{eq} as a function of V_{KOH}(mL).

a) (10 pts) Determine the pOH of the solution as a function of the volume of KOH solution added.

b) (20 pts) Create a graph which has plots of pH and pOH as a function of KOH solution added. Estimate the volume of the KOH solution required to reach the equivalence point of this titration. Estimate the molar concentration of the initial nitric acid solution.

c) (20 pts) Actually, the initial concentration of the nitric acid can be determined at each volume of the added KOH solution. Use a computer program/spreadsheet to calculate the initial concentration of HNO_3 from the pH data at each volume of added base.

d) (30 pts) Another method to obtain the initial concentration of the nitric acid is by curve-fitting the data. Use the user-defined function of the Regression Wizzard curve- fitting feature of SigmaPlot to obtain the initial concentration of nitric acid. Be sure to describe in detail how you did this.

Titration of Strong Acid by Strong Base

For the case where aVa>bVb

	$2H_2O(l) \Longleftrightarrow$	$H_3O^+(aq)$ +	$OH^-(aq)$	$K_w = [H_3O^+][OH^-]$
$[\ ]_{init}$	-----	$\frac{a\,V_a}{V_a+V_b}$	$\frac{b\,V_b}{V_a+V_b}$	assuming volumes are additive
$\Delta[\ ]$	-----	$\frac{-b\,V_b}{V_a+V_b}$	$\frac{-b\,V_b}{V_a+V_b}$	
$[\ ]_{new}$	-----	$\frac{a\,V_a - b\,V_b}{V_a+V_b}$	0	$Q = 0$; $Q < K_w$
$\Delta[\ ]$	-----	$+X$	$+X$	
$[\ ]_{eq}$	-----	$\frac{a\,V_a - b\,V_b}{V_a+V_b} + X$	X	

where a and b are the concentrations of the strong acid and base before mixing respectively; Va and Vb are the volumes of the strong acid of concentration a and strong base of concentration b that are mixed together. Therefore:

$$K_w = \left(\frac{(a\,V_a - b\,V_b)}{(V_a+V_b)} + X\right)(X) = \frac{(a\,V_a - b\,V_b)}{(V_a+V_b)}X + X^2$$

$$0 = X^2 + \frac{(a\,V_a - b\,V_b)}{(V_a+V_b)}X - K_w$$

For $(a\,V_a > b\,V_b)$ $\quad X = (-((a\,V_a - b\,V_b)/(V_a+V_b)) + (((a\,V_a - b\,V_b)/(V_a+V_b))^2 + 4K_w)^{1/2})/2$

It is left to the student to show that

For $(a\,V_a < b\,V_b)$ $\quad X = (-((b\,V_b - a\,V_a)/(V_a+V_b)) + (((b\,V_b - a\,V_a)/(V_a+V_b))^2 + 4K_w)^{1/2})/2$

Titration of Weak Acid by Strong Base

For the case where aVa>bVb

	$A^-(aq)$	$+ H_2O(l)$ <===>	$HA(aq)$	$+ OH^-(aq)$	$K_b = (K_a/K_w) = [HA][OH^-]/[A^-]$
$[\ ]_{init}$	0	-----	$\frac{a\,V_a}{V_a+V_b}$	$\frac{b\,V_b}{V_a+V_b}$	assuming volumes are additive
$\Delta[\ ]$	$\frac{b\,V_b}{V_a+V_b}$	-----	$\frac{-b\,V_b}{V_a+V_b}$	$\frac{-b\,V_b}{V_a+V_b}$	
$[\ ]_{new}$	$\frac{b\,V_b}{V_a+V_b}$	-----	$\frac{a\,V_a - b\,V_b}{V_a+V_b}$	0	$Q = 0;\ Q < K_b$
$\Delta[\ ]$	-X	-----	+X	+X	
$[\ ]_{eq}$	$\frac{b\,V_b}{V_a+V_b} - X$	-----	$\frac{a\,V_a - b\,V_b}{V_a+V_b} + X$	X	

where a and b are the concentrations of the weak acid and strong base before mixing respectively; Va and Vb are the volumes of the weak acid of concentration a and strong base of concentration b that are mixed together. Therefore:

$$K_b = \left(\frac{(aV_a - bV_b)}{(V_a+V_b)} + X\right)(X) \,/\, ((bV_b/(V_a+V_b)) - X)$$

$$0 = X^2 + \left(\frac{(aV_a - bV_b)}{(V_a+V_b)} + K_b\right)X - K_b(bV_b/(V_a+V_b))$$

For $(aV_a > bV_b)$ $$X = (-((aV_a - bV_b)/(V_a+V_b) + K_b) + (((aV_a - bV_b)/(V_a+V_b) + K_b)^2 + 4K_b\, bV_b/(V_a+V_b))^{1/2})/2$$

It is left to the student to show that

For $(aV_a < bV_b)$ $$X = (-((bV_b - aV_a)/(V_a+V_b) + K_b) + (((bV_b - aV_a)/(V_a+V_b) + K_b)^2 + 4K_b\, aV_a/(V_a+V_b))^{1/2})/2$$

and

For (aVa = bVb) $$X = (- K_b + ((K_b)^2 + 4K_b\, bV_b/(V_a+V_b))^{1/2})/2$$

Sigma Plot Transform Commands

col(*i*)	*i*th column
cell(c,r)	cell in row r, column c

for I=1 to n step w do
statement(s)
end for
	loop from 1 to n in steps of w. Step w optional.

If *argument* then
statement(s)
else
statement(s)
end if
	Conditional statements performed if argument is true.
	Else is optional

log(x)	Common log of x.
10^-x	anti-common log of -x
N^z	N raised to the power of z
sqrt(x)	square root of x

Other functions found under Transform Commands in Contents of Help

	Vol KOH	pH
1	1.0000	0.9394
2	2.0000	1.0024
3	3.0000	1.0664
4	4.0000	1.1323
5	5.0000	1.2009
6	6.0000	1.2733
7	7.0000	1.3510
8	8.0000	1.4359
9	9.0000	1.5311
10	10.0000	1.6413
11	11.0000	1.7751
12	12.0000	1.9508
13	13.0000	2.2191
14	14.0000	2.9028
15	15.0000	11.5052
16	16.0000	11.8662
17	17.0000	12.0502
18	18.0000	12.1719
19	19.0000	12.2616
20	20.0000	12.3318
21	21.0000	12.3889
22	22.0000	12.4367
23	23.0000	12.4775
24	24.0000	12.5129
25	25.0000	12.5440