

Integrating Good Figures and Good Tables in Text in CH 462

Examples of student writing are from Experimental Chemistry II, CH 462, a required WIC and advanced laboratory course for many chemistry majors. Mike Lerner and I are co-instructors for the course and the enrollment is usually 12-18 junior and senior level chemistry majors. Students work in groups of 2-3 on four projects winter term. At the first class students are given directions verbally and in writing on expectations for writing reports (handout, "Class Requirements and Grading Policies", also posted online). The ACS Style Guide text is required and we encourage students to read professional ACS published papers for examples on how and what to write. They receive feedback on their reports in writing and we meet with each student and go over the feedback in person for report 1 during class (report day). Students revise report 1 and resubmit, and new this year we added a peer review on report 1, which led to a third revision. Examples given today are from the last report of the term due during finals week.

For Figures and Tables in a report, order is important and proximity to use in text. Some common problems that we usually encounter for both of these elements are, for example:

- Not numbered
- Missing caption/legend or caption/legend not descriptive
- No reference in text to Table/Figure X, and/or reference out of order in text

In addition, for Scientific Tables:

- Redundant data /results given in many tables
- Too many significant figures that make tables too busy (not good science)
- Insignificant data /results given status of a table!
- Units and abbreviations are not given in column headings
- Entries not centered under headings (spreadsheets cause issues)
- Don't fit on one page and are not adequately labeled on second page

and Scientific Figures:

- Too many or too few significant figures on axes labels (not good science)
- General errors in figure format or units missing or redundant
- Calling figures charts/graphs/schemes, e.g.

Let's look at some examples

Table II. Recovery of Fat-Soluble Vitamins A, D₃, and E in Animal Feeds^{a, b}

sample	unspiked			spiked			found			% recov.		
	A	D ₃	E	A	D ₃	E	A	D ₃	E	A	D ₃	E
dairy supplement	2739		39	3803	100000	50	6523	88000	91	99	88	97.5
mineral feed, special vitamins	3258		11	1153	40000	20	4629	40000	28.5	96	100	97.7
protein sow supplement	5919		50	761	40000	10	6524	36000	58.5	97	90	92.5
dairy supersweet mix	982			1523		20	2456		18.5	98		92.5
all mash layer (14%)	1184		13.5	3808	100000	50	4892	87000	57.5	93	87	90.5

^a Vitamin A represents vitamin A acetate or palmitate or both of them. D₃ was not present. E represents E acetate or E alcohol or both of them. The overall percent recoveries of D₃ in feed are 91.25 ± 5.9 ; of A, 96.4 ± 2.4 ; of E, 92.6 ± 2.92 .

^b The vitamins are expressed as IU/kg.

Table III. Comparison of AOAC and LC Method for Vitamin A, D, and E^a

	guarantee			AOAC method ^b			LC method		
	A	D ₃	E	A	D ₃	E	A	D ₃	E
pre-mix mineral	220		220	296		236	301		215
pre-mix for turkey and pig	35723	3527	88	36919		73.4	32983	2900	68
pre-mix for poultry	7709	1651	7700	7966		6600	7518	1693	7230
feed (cattle)	285		385	348		273	297		328
feed (rabbit)	18931		44	18000		38	17770		35
feed (horse)	11000		11	10000		10	9953		10

^a The vitamin A is either vitamin A acetate, A alcohol, or A palmitate, or the sum of two or three of them; vitamin E is either E acetate or E alcohol or the sum of these two. Vitamins are expressed as IU/kg, except for pre-mix samples which are IU/g. ^b For vitamin D₃, the AOAC method was not available in our laboratories.

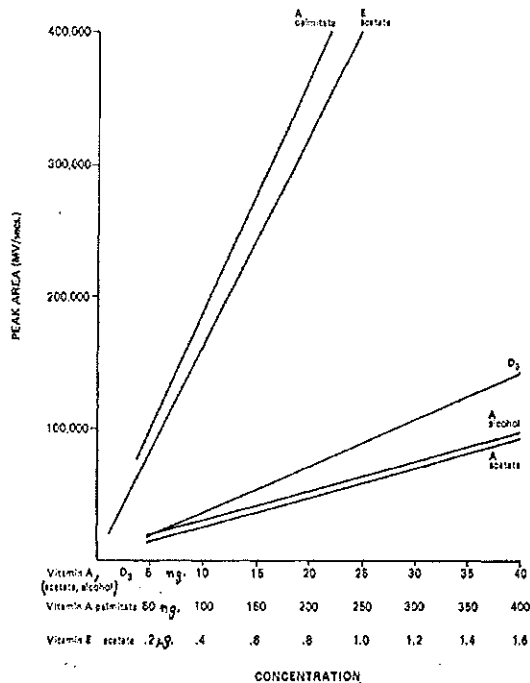


Figure 3. Linear dynamic range of the five vitamins.

and 60 ng of vitamin A palmitate can be detected. The discrepancy in half-scale response of the vitamins A and E is due to the much lower extinction coefficient of the latter. But the linear dynamic range is adequate for most problems of quantitative analysis of all three vitamins.

Recovery studies were performed on five different samples from various sources. Blanks were run in triplicate on all samples prior to spiking to determine levels of vitamins. No peaks were found to interfere with either vitamin A, D, or E. The quantities of vitamin spiked are summarized in Table II. Minimum detectable amounts are: vitamin A, 250 IU/kg; vitamin D₃, 10 000 IU/kg; vitamin E, 5 IU/kg.

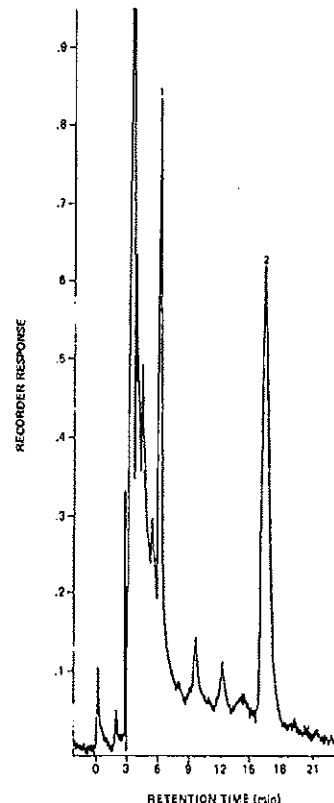


Figure 4. High-pressure liquid chromatography of vitamin A acetate (peak 1) and vitamin E acetate (peak 2) in a 10-g feed sample. UV detector sensitivity setting, 0.005 a.u.

The recovery percentages are the following: vitamin A acetate, 96.4 ± 2.4 ; vitamin D₃, 81.25 ± 5.9 ; vitamin E acetate, 92.6 ± 2.92 .

Figure 4 is the chromatogram of a feed sample (10 g) using the method previously described. Elution is from a μ Bondapak/C₁₈ column with methanol-water (95:5) at

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Once again the term in Equation 7 involving other species is assumed to be comprised of only the $\text{Fe}(\text{SCN})_2^+$ complex. Furthermore, Equation 4 can be rewritten to find a total amount of iron tied up in SCN^- complexes.

$$T_{\text{Fe}/\text{SCN}} = T_{\text{Fe(III)}} - [\text{Fe}^{3+}] - [\text{FeOH}^{2+}] \quad (8)$$

①
well done

Combination of Equations 7 and 8 yields:

$$[\text{SCN}^-] = T_{\text{SCN}} - T_{\text{Fe}/\text{SCN}} \quad (9)$$

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The quantities $[\text{Fe}^{3+}]$, $[\text{FeOH}^{2+}]$, T_{SCN} , and $[\text{SCN}^-]$ were calculated at each titration point and are summarized in Table 2.

Volume KSCN (μL)	E_{cell} (V)	T ($^{\circ}\text{C}$)	T_{SCN}	$[\text{Fe}^{3+}]$	$[\text{FeOH}^{2+}]$	$[\text{SCN}^-]$	Q
0	0.4946	22.5	0.0000	9.81E-04	1.85E-05	0.00E+00	0.0
100.7	0.4862	22.5	0.0020	7.08E-04	1.34E-05	1.74E-03	227.1
201.4	0.4792	22.5	0.0040	5.38E-04	1.02E-05	3.58E-03	235.1
302.1	0.4732	22.5	0.0060	4.25E-04	8.03E-06	5.47E-03	243.8
402.8	0.4680	22.5	0.0081	3.46E-04	6.55E-06	7.41E-03	252.0
503.5	0.4632	22.5	0.0101	2.87E-04	5.42E-06	9.36E-03	263.4
604.2	0.4590	22.5	0.0121	2.43E-04	4.60E-06	1.13E-02	272.7
704.9	0.4551	22.5	0.0141	2.09E-04	3.95E-06	1.33E-02	283.2
805.6	0.4515	22.5	0.0161	1.81E-04	3.43E-06	1.53E-02	294.0

Table 2. Data and calculated species concentrations and for each point in the titration of a $9.81 \times 10^{-4} \text{ M Fe}^{3+}$ and $2.00 \times 10^{-4} \text{ M Fe}^{2+}$ solution with 2.000 M KSCN

Using the expressions for both β_1 and β_2 the following relationship can be derived (see Supplemental Information for full mathematical treatment):

$$Q = \beta_1 + \beta_2[\text{SCN}^-] \quad (10)$$

④
good legend

where $Q = T_{\text{Fe}/\text{SCN}} / [\text{Fe}^{3+}] (T_{\text{SCN}} - T_{\text{Fe}/\text{SCN}})$. Therefore, a plot of Q versus $[\text{SCN}^-]$ should be linear with a slope of β_2 and a y-intercept of β_1 . Such a plot is shown in Figure 2 yielding β_1 and β_2 values of 217 M^{-1} and 4950 M^{-2} respectively.

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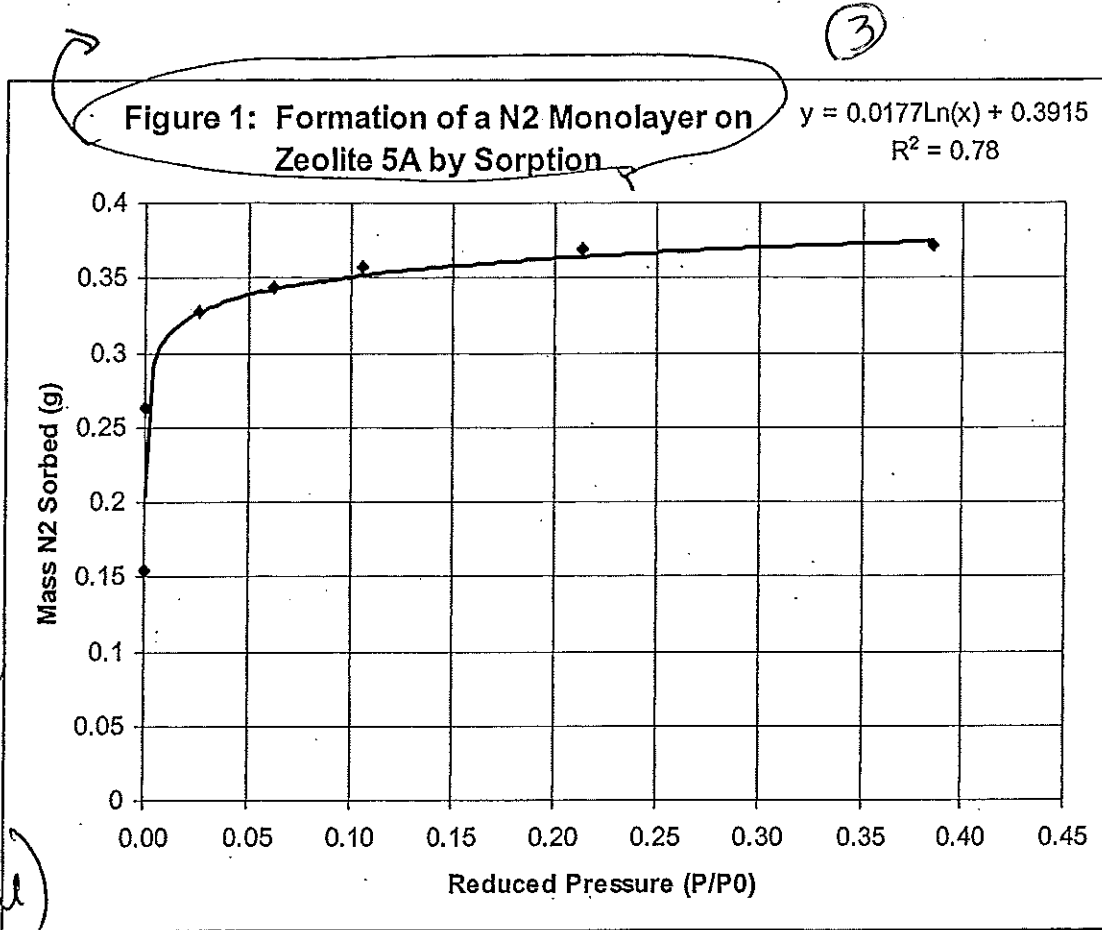
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Zeolite 5A will be able to be calculated. Figure 1 shows the formation of the N₂ monolayer on the Zeolite 5A.

N ₂ Pressure (torr)	Reduced Pressure	Sample Mass (g)	Total Mass N ₂ Sorbed (g)
292	0.384	0.9042	0.3718

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the ACS
style guide)



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Supplemental Information:

Part A:

Limiting Reagents

Zeolite 4A Na₂SiO₃ · 9H₂O = 10g 10g * MW Na₂SiO₃ · 9H₂O = 0.035 mol

NaAlO₂ = 8g 8g * MW NaAlO₂ = 0.098 mol

1

2 Due to its larger scanning range Figure 3 shows both of the reduction waves of oxygen (Table 3). A reversible reaction has a potential range of ~ 0.15 V while an irreversible reaction has a larger range⁴. Since the second wave extends over a significantly larger potential range (~ 0.9 V) than the first wave (~ 0.1 V) it can be seen that the first wave is a reversible reaction, while the second is an irreversible reaction.

The concentration of oxygen in the solution, which was 21°C , was determined to be 0.2542mM (0.00813 g/L) (Appendix D). This value is 8.65% different from the literature value of 0.0089 g/L .³

good value

Figure 3: Sampled dc polarogram showing voltage vs current for a solution of 0.1M KNO_3 scanning from 0.2V to -1.8V at 5 mv/s and 25 samples/s with a current range of $10\mu\text{A}$. (Run 3)

3

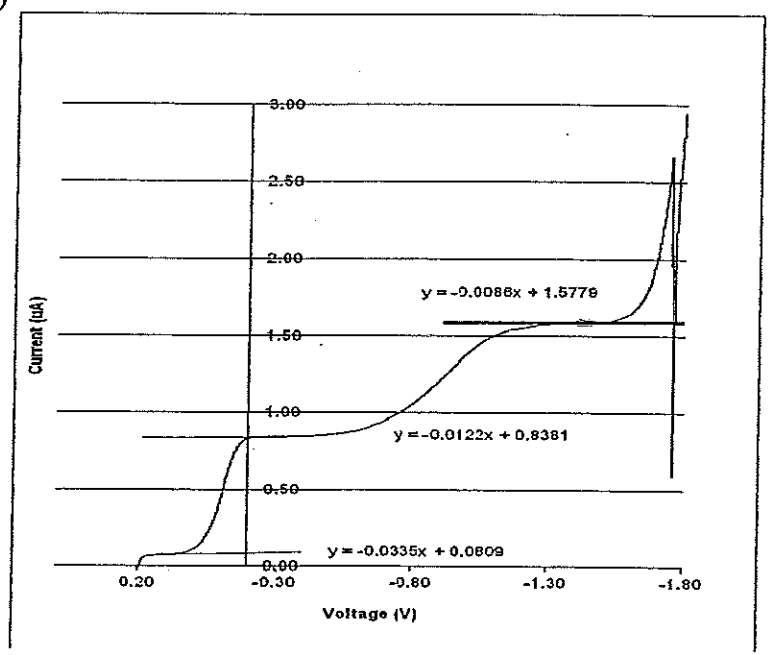


Table 3: Electrode reactions, diffusion currents, and half-wave potentials for oxygen waves in Figure 3.

Wave	Electrode Reaction	i_d	$E_{1/2}$
1	$\text{O}_2 + 2\text{H}^+ + 1\text{e}^- \rightarrow \text{H}_2\text{O}_2$	0.7479	-0.108
2	$\text{H}_2\text{O}_2 + 2\text{H}^+ + 1\text{e}^- \rightarrow 2\text{H}_2\text{O}$	0.7348	-0.905

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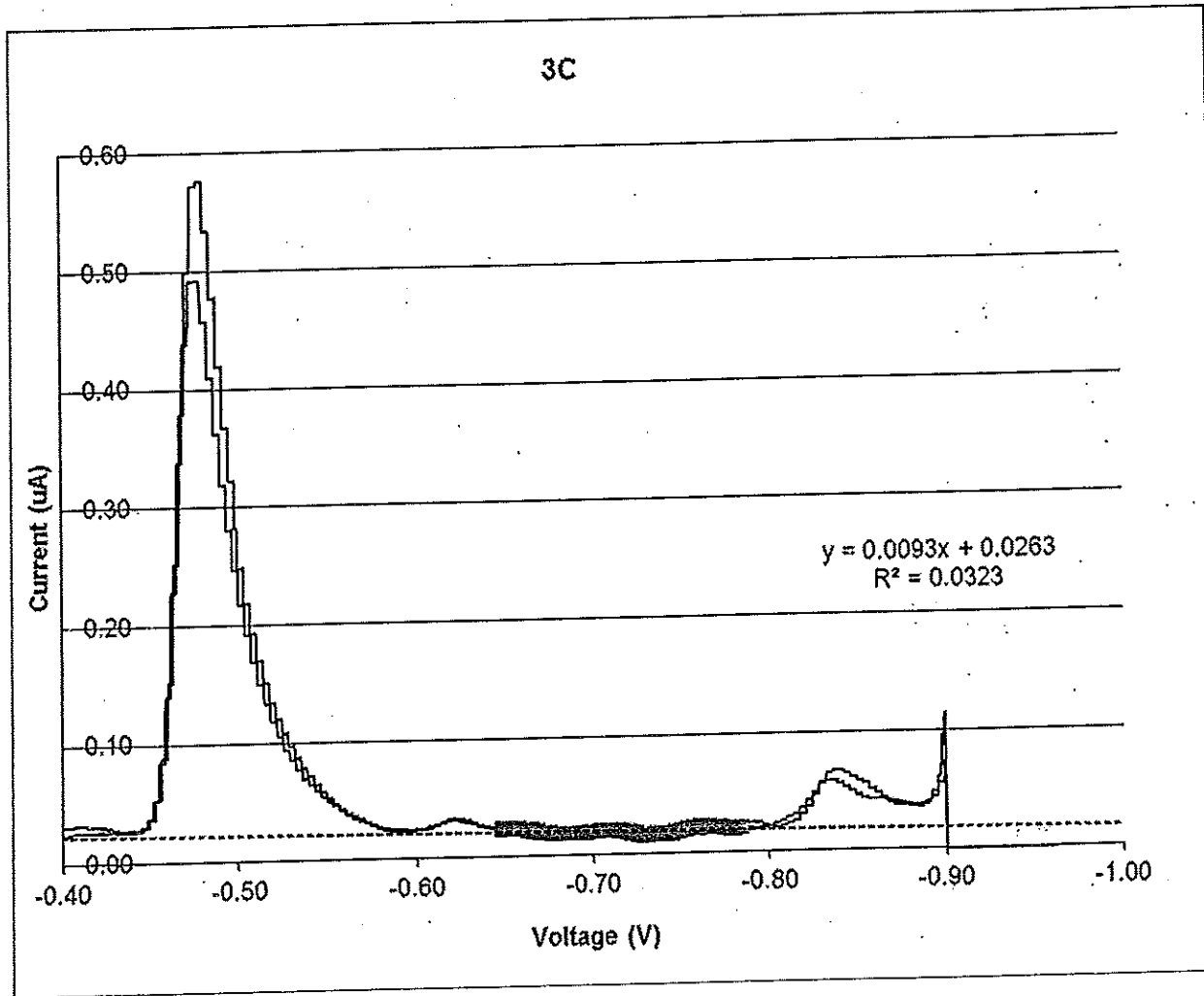


Chart 4 : 3C

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trendline regression was applied to the used data range. Figures 9-12 represent the logarithmic plots of the decay curves for Solutions 1-4, respectively.

Solution	[H ⁺] (M)	Run	k(obs)		Avg k(obs)
			L/mol*ms	Δk(obs)	
1	0.1024	1	1.53E-03	1.53E-05	1.60E-03
		2	1.60E-03	1.78E-05	
		3	1.67E-03	2.04E-05	
2	0.06144	1	1.77E-03	1.87E-05	1.74E-03
		2	1.50E-03	1.49E-05	
		3	1.95E-03	1.83E-05	
3	0.04096	1	3.56E-03	3.25E-05	3.55E-03
		2	3.54E-03	2.83E-05	
4	0.02048	1	4.80E-03	5.23E-05	4.95E-03
		2	4.93E-03	6.13E-05	
		3	5.13E-03	4.59E-05	

Table 4: Flash photolysis results showing [H⁺], k_{obs}, uncertainty for k_{obs} and avg. k_{obs} for each solution.

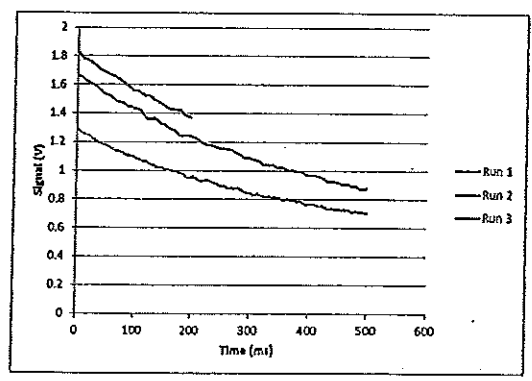


Figure 5: Decay curve for [H⁺] = 0.1M.

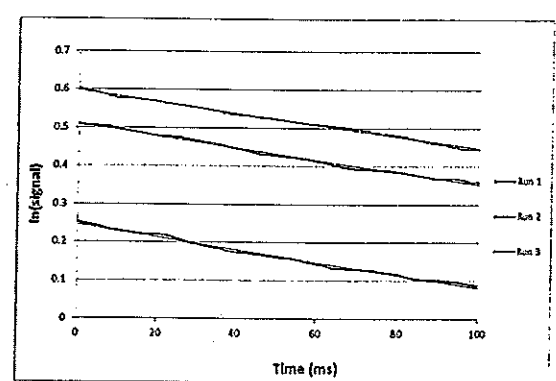


Figure 9: Logarithmic plot for [H⁺] = 0.1M

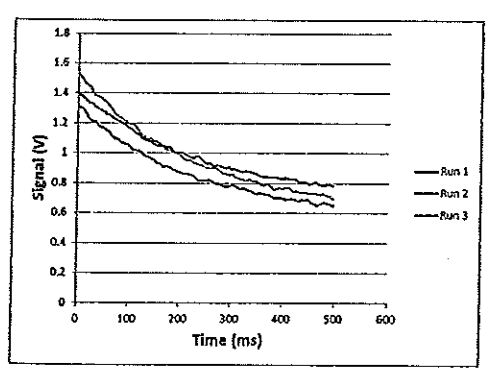


Figure 6: Decay curve for [H⁺] = 0.06M.

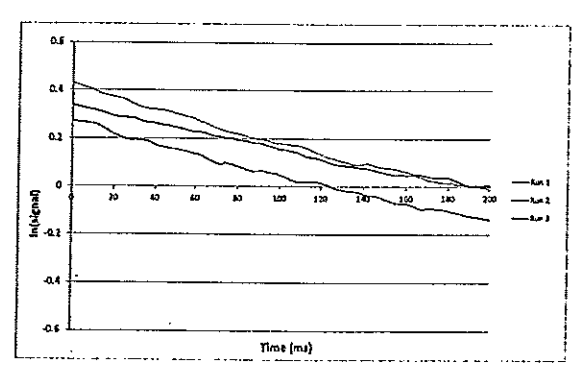


Figure 10: Logarithmic plot for [H⁺] = 0.06M

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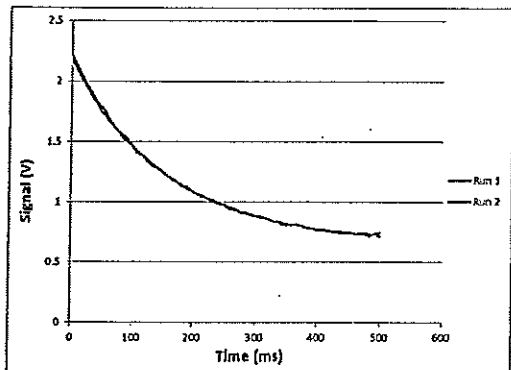


Figure 7: Decay curve for $[H^+] = 0.04M$.

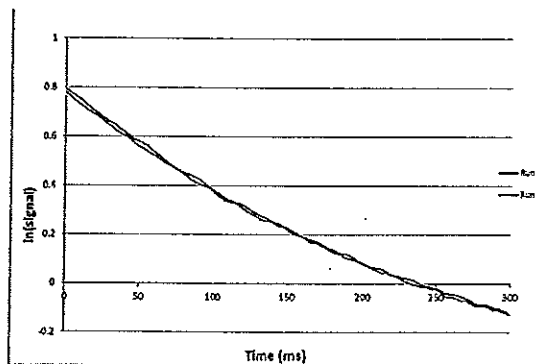


Figure 11: Logarithmic plot for $[H^+] = 0.04M$

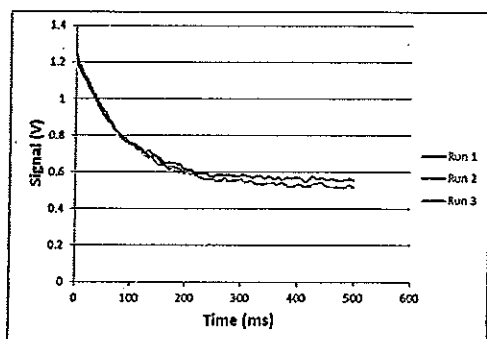


Figure 8: Decay curve for $[H^+] = 0.02M$.

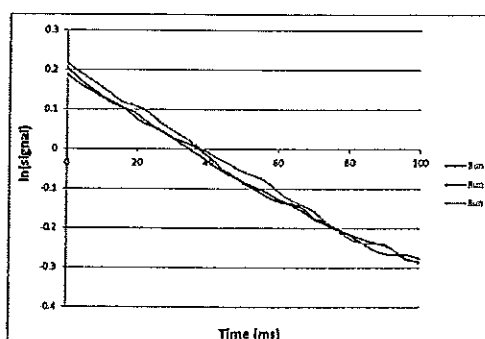


Figure 12: Logarithmic plot for $[H^+] = 0.02M$

As shown in the decay curves and in Table 4, k_{obs} increased as $[H^+]$ decreased. The error (Δk_{obs}) associated to k_{obs} was the st. dev. obtained from linear regression. The average k_{obs} was taken as the experimental value for each solution. It should be noted that the units for k_{obs} were $Lmol^{-1}(ms)^{-1}$.

A plot of k_{obs} vs $1/[H^+]$ was used to determine the rate constants (k_{12} , k_{34}) and g for the individual reactions as explained in the literature^[8]. Equation 3 shows the mathematical relationship employed and the graph is found in Figure 13. There was a relatively linear relationship, which enabled a linear regression to be used to determine the equation.

$$(3) k_{obs} = k_{34}K_h g / [H^+] + k_{12}g \quad K_h = 0.00189$$

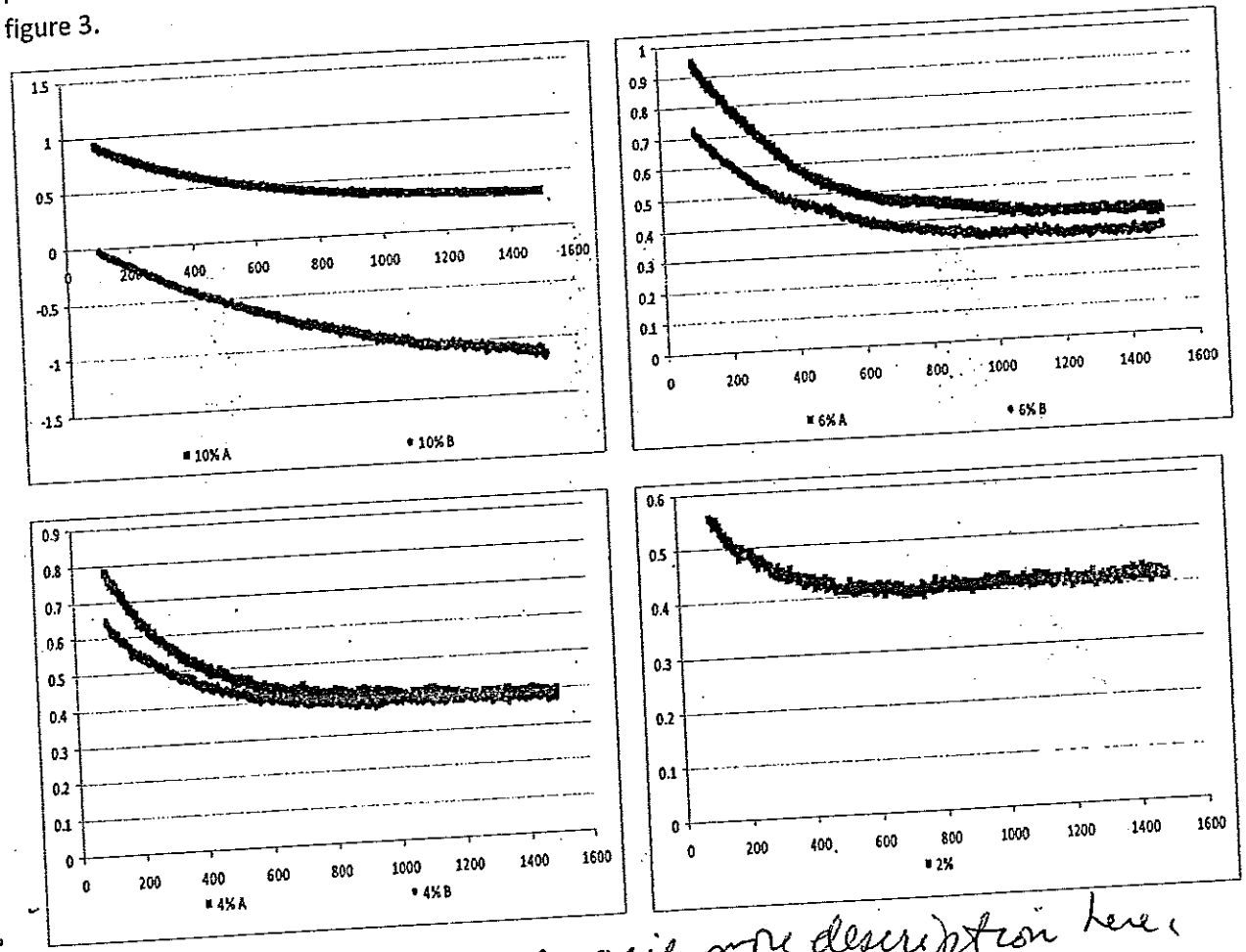
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From this plot, the equilibrium constants β_1 and β_2 can be gleaned, and were found to be $\beta_1 = 196 \pm 10$ and $\beta_2 = 1.48 \times 10^4 \pm 1.0 \times 10^3$. From these two values, $K_1 = \beta_1 = 196 \pm 10$, and $K_2 = \beta_2 / \beta_1 = 75.5 \pm 6.4$. These values compare to literature values of $K_1 = 139$ and $K_2 = 20.4$.² Both of these values are higher than the literature values, but as expected, the K_2 value is lower showing that the formation of higher order complexes of ferric thiocyanate form slower than the 1:1 complex, which agrees with the stoichiometry reported above.

*This is not kinetics, this is thermodynamics
 $\Delta G = -RT \ln K$*

4. Kinetic Study of Complex Formation.

After the stoichiometry had been determined along with the equilibrium constants, the natural progression is to next determine the kinetics of the complex formation. In order to achieve this, flash photolysis was used employing a relaxation kinetic study. The decay curves for this study are found in figure 3.



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Figure 3. Decay curves of kinetic study. *← give more description here.*

The upper right hand graph is the curve found for the solution containing 0.10 M hydrogen ion concentration, the upper left is 0.06 M $[H^+]$, the lower right is 0.04 M $[H^+]$ and the lower left is 0.02 M $[H^+]$. All data was obtained over 1500 ms after the solution had been bleached with a camera flash source. From the raw data in figure 3, the plots in figure 4 were constructed by plotting the natural log

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Results and Discussion

Part A - Potentiometry

For this part, two voltages were measured using a three compartment electrochemistry cell. The first was of a 0.09M KNO_3 and 0.01M KCl solution saturated with 0.1M $AgNO_3$, and was measured to be 103.0 mV. This fit perfectly with expected value^[2]. The second voltage measured was of a 0.09M KNO_3 and 0.01M $AgNO_3$ solution, and was found to be 419.2 mV, slightly lower than the expected value^[1]. More information about each run is presented in Table 1.

This information is mainly given above we need for table

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Solution	E_{cell} (mV)	Uncertainty	Ionic Strength	Temp. (°C)	$E_{SCE}^{[2]}$
KCl	103.0	+/- 1.0 mV	0.10 M	22.0	0.243
$AgNO_3$	419.2	+/- 1.0 mV	0.10 M	22.0	0.243

Table 1: Electrochemistry Cell Data

From the data in the table above, the values for $E_{Ag^+/Ag}$ and $E_{AgCl/Ag}$ were calculated using Eq 12 and 15 from the lab manual^[3], using the assumption that E_{ij} is zero. $E_{Ag^+/Ag}$ was found to be 0.6622V, while $E_{AgCl/Ag}$ was found to be 0.3442V. Had E_{ij} been non-zero but equal for each solution, the answers would both be off by the same amount, as E_{ij} was simply a constant that was added to them. If E_{ij} was different for each solution, then there would be a bigger difference, which would more greatly effect the accuracy of the data.

where is E^0 ?
if this is $E_{Ag^+/Ag}$
this value is low

Using equation 18 from the manual^[3], the value for μ for each solution was found to be 0.1.

From this, equation 17^[3] can be used to find γ for each solution. Using the values presented in the manual^[3] for A and B, γ_{Ag} was found to be 0.880 and γ_{Cl} was 0.885. From this and the known concentration being multiplied together as described in equation 16^[3], a_{Ag} was found to be 0.088 and a_{Cl} was found to be 0.089.

These values are not typical

The values given in the lab manual for the γ for each solution was significantly lower (~10%)

where are your sample calculations?

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$$[FeOH^{2+}] = \frac{K_h[Fe^{3+}]}{[H^+]} \quad (3)$$

Logarithmic decay curves for multiple photolysis runs at four acid concentrations are shown in Figures 2.1 through 2.4 in the Appendix. From each decay plot the k_{obs} was determined using (4), where t is time in milliseconds, and can be found in Table 4. The average k_{obs} , (Table 5) from each concentration are plotted in Figure 3 as a function of $1/[H^+]$.

$$\ln\left(\frac{[x]_t}{[x]_{t=0}}\right) = -k_{obs}t \quad (4)$$

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Figure 3. Linear Regression of The Observed Rate

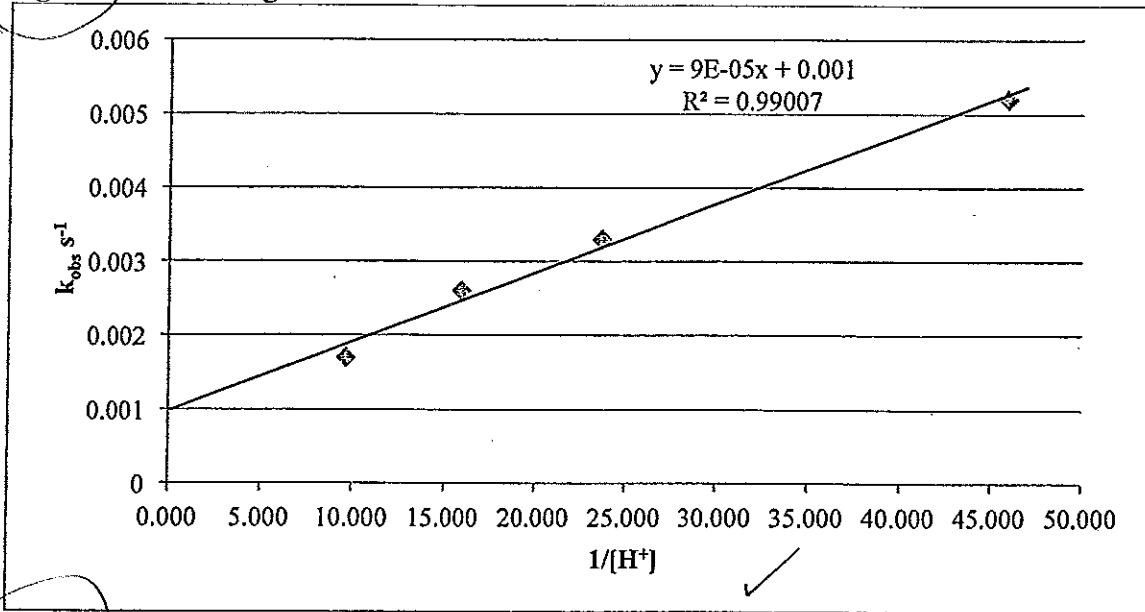


Figure 3. Above, the linear regression of the observed rate constant k_{obs} , as function of inverse acid concentration and linearity begins to decline as concentration increases (where $1/[H^+]$ is ~ 9.6).

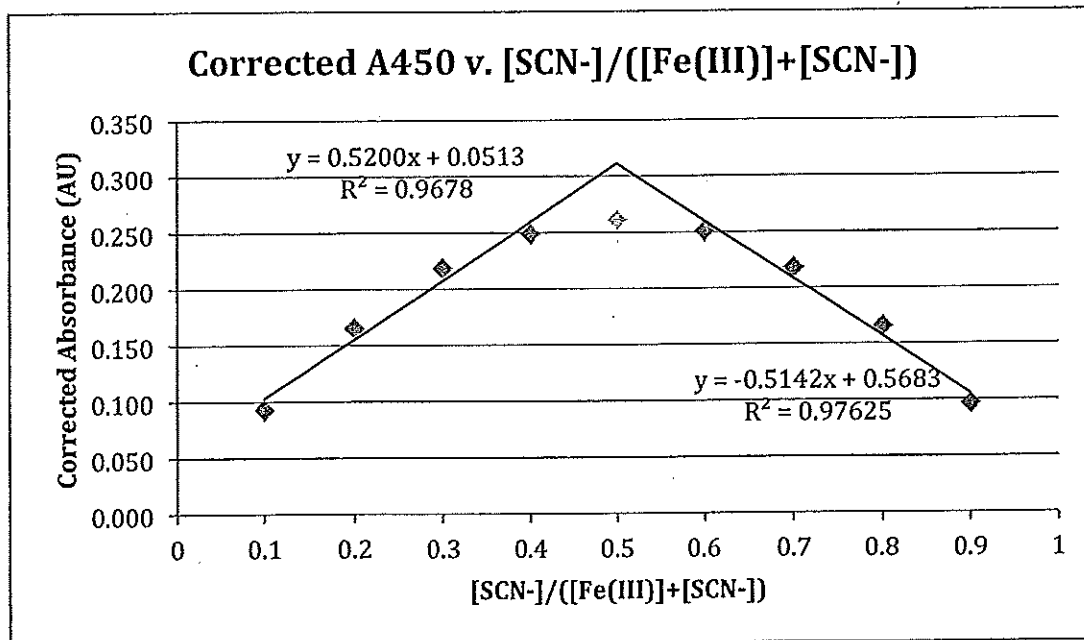
Table 4. k_{obs} For Individual Runs at Different H^+ Concentrations

0.02 M	$k_{obs} s^{-1}$	Average	Deviation	0.06 M	$k_{obs} s^{-1}$	Average	Deviation
Run 1	0.0049	0.0052	0.0004	Run 1	-	0.0026	0.0003
Run 2	0.0048			Run 2	0.0028		
Run 3	0.0057			Run 3	0.0023		
Run 4	0.0054			Run 4	0.0028		
0.04 M	$k_{obs} s^{-1}$	Average	Deviation	0.10 M	$k_{obs} s^{-1}$	Average	Deviation
Run 1	0.003	0.0033	0.0003	Run 1	0.0017	0.0017	0.0001
Run 2	0.0034			Run 2	0.0018		
Run 3	0.003			Run 3	0.0018		
Run 4	0.0036			Run 4	0.0015		

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TABLE 5 NEXT P.

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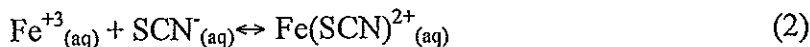
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Figure 2-A plot of the corrected absorbance versus $[\text{SCN}^-]/([\text{Fe(III)}]+[\text{SCN}^-])$ based on the linear extrapolation of the two sides of the peak from Figure 1. The two linear extrapolation lines intersect at the maximum absorbance.

Figure 2 demonstrates that the maximum absorbance of the complex occurred when the two components were in equal volumes, which means the mole fraction for the two reactants was 0.5. Based on the linear extrapolations seen in Figure 2, the maximum absorbance occurs at 0.31125 AU. The two linear extrapolation lines in figure 2 intersect at 0.499903, which corresponds to the maximum absorbance measured experimentally having its maximum at 0.5 for $[\text{SCN}^-]/([\text{Fe(III)}]+[\text{SCN}^-])$. The maximum absorbance occurring where the reactants are in a 1:1 ration indicates the reaction has the stoichiometry:



Initially, equation 1 was the starting point and when the relationship of the reactants was determined to be 1:1, the value of 1 was inserted into equation 1 for all of the n variables.

Equilibrium Constant for the Complex

All sample calculations for this experiment can be found in Appendix C.

The purpose of the equilibrium constant complex experiment was to determine the equilibrium constant for:

