

Investigation of the Relationship between Temperature and Equilibrium Constant of a Thiocyanatoiron Complex Reaction

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1 Introduction

As someone who wants to major in Control Theory, the field of engineering that deals with the control of dynamic systems and processes, I have always been fascinated by industrial chemical processes like the Haber-Bosch Process and the Fischer-Tropsch Process. Specifically, I have always wondered how chemical engineers have optimized the efficiency and yield of these processes by selectively choosing the temperature and pressure conditions for the reaction.

In my chemistry class, I learned about how Le Chatelier's principle could be applied to shift the chemical equilibrium towards a desired product. However, I soon realized that knowing which product is thermodynamically favored is only one factor among many such as reaction rate and practical feasibility that chemical engineers must consider. Chemical engineers must realize the relationship between the temperature and equilibrium constant to find the precise temperature compromise to precisely optimize for all such factors (Clark, 2022). Hence, I decided to explore how temperature affects the equilibrium constant for a thiocyanatoiron complex reaction for my Chemistry Internal Assessment.

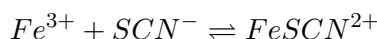
1.1 Research Question

What is the relationship between the equilibrium constant and temperature of a thiocyanatoiron complex reaction?

2 Background Research

2.1 Primary Reaction

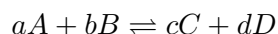
This experiment will use the thiocyanatoiron complex reaction as a means to explore the relationship between the equilibrium constant and temperature. The complex formation reaction is described below (Nazareay, 2020).



2.2 Equilibrium Constant

The equilibrium constant (K_c) is a measure of the extent to which a chemical reaction proceeds to completion. It is defined as the ratio of the concentrations of the products to the concentrations of the reactants, each raised to the power of their respective stoichiometric coefficients. The equilibrium constant is a crucial parameter in understanding the position of equilibrium in a chemical reaction. If $K_c < 1$, the equilibrium favors the creation of reactants. If $K_c > 1$, the equilibrium favors the creation of products. (Hammett, 1935)

For a reaction:



The equilibrium constant can be calculated as follows:

$$K_c = \frac{[C]^c \times [D]^d}{[A]^a \times [B]^b} \quad (1)$$

2.3 Colorimetry

Colorimetry is a technique to determine the concentration of a substance in a solution by measuring the absorbance of monochromatic light using a spectrophotometer. It is based on the principle that different substances absorb and transmit light at different wavelengths. By comparing the absorbance of a sample to that of a standard solution, the concentration of the substance in the sample can be determined using the Beer-Lambert Law described below. Colorimetry is widely used in various fields, including environmental analysis, clinical chemistry, and industrial quality control, due to its simplicity, speed, and accuracy (Clydesdale and Ahmed, 1978).

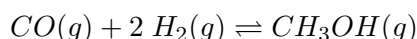
$$A = \epsilon b C \quad (2)$$

Where:

- A is the absorbance (%).
- ϵ is the molar absorptivity ($M^{-1} \text{ cm}^{-1}$).
- b is the path length (cm).
- C is the molar concentration of the colored sample (M).

2.4 Importance of Knowing How Temperature Changes the Equilibrium Constant

Understanding how temperature changes the equilibrium constant of a reaction is crucial for predicting and controlling chemical reactions. The following reaction describes the synthesis of methanol from carbon monoxide and hydrogen gas.



The reaction is exothermic, meaning it releases heat ($\Delta H < 0$). According to Le Chatelier's principle, for exothermic reactions, the equilibrium constant K_c decreases with increasing temperature. This means that at higher temperatures, the reaction will shift towards the reactants, producing less methanol. Conversely, at lower temperatures, the reaction will shift towards the products, producing more methanol.

Therefore, in the industrial production of methanol, it would be more beneficial to run the process at a lower temperature to maximize the yield of methanol. However, it's important to note that while lower temperatures favor the production of methanol in terms of thermodynamics, reaction rates are typically slower at lower temperatures. Therefore, a compromise temperature of 250 degrees Celsius is often chosen in industry to balance the thermodynamic favorability with a reasonable reaction rate. Thus, knowledge of how temperature affects the equilibrium constant is essential for optimizing industrial processes and ensuring efficient production of desired products (Gallucci, 2018).

3 Hypothesis

If the temperature of the solution increases, then the equilibrium constant of the reaction will decrease exponentially. If the temperature of the solution decreases, then the equilibrium constant of the reaction will increase exponentially.

4 Variables

4.1 Independent Variables and Dependent Variables

The independent variable for this experiment is the temperature of the solution, which is measured by a Vernier Temperature Probe with a precision of $\pm 0.1^\circ\text{C}$. The dependent variable for my experiment is the absorbance of a monochromatic light source of the thiocyanatoiron(III) complex ion in the reaction, which is measured using a spectrophotometer with a precision of ± 0.00035 transmittance. The transmittance will be used to derive the concentration of the thiocyanatoiron(III) complex ion and thus the equilibrium constant of the reaction. More details about the specific measurement processes are described in the Section 6.

4.2 Control Variables

I ensured that all other variables were controlled to get accurate results about the relationship between the equilibrium constant and temperature. For example, throughout the trials, the solution remained untouched so that no variations would occur due to the slight variations in the initial concentrations of Fe^{3+} and SCN^- . Furthermore, the same amount of water (200 mL) at roughly the same initial temperature ($< 20^\circ\text{C}$) was used for every trial with the same heating source to ensure that the controlled temperature increased at the same rate throughout the trials. Finally, the beaker, temperature probe, and thermistor were always cooled down to room temperature before proceeding to do a new trial. Through all measures, a more accurate relationship between my independent and dependent variables can be assessed.

5 Methodology

5.1 Materials

- Vernier Temperature Probe, $\pm 0.1^\circ\text{C}$
- GoLink (for connecting to Logger Pro)
- Logger Pro Software on Laptop (for dynamic temperature logging)
- Spectrophotometer (for use in colorimetry), $\pm 0.01\%$
- 1.2 cm Square Cuvettes (to hold spectrophotometer sample)
- Hot Plate (as heat source)
- 400 mL Glass Beaker
- Beaker Tongs and Wire Gauze (to handle hot beaker)
- Forceps (to move hot cuvettes)
- $\text{Fe}(\text{NO}_3)_3$ Solution, 0.100 M
- KSCN Solution, 0.001 M
- $\text{Fe}(\text{NO}_3)_3$ Solution, 0.025 M
- KSCN Solution, 0.025 M
- Deionized Water

6 Procedure

Create a blank DI water sample for spectrophotometer calibration. Create the standardization samples as per Table 1 and fill a cuvette with each. Record the transmittance for each standardization sample.

Volume of 0.1M $Fe(NO_3)_3$ (mL)	Volume of 0.001M $KSCN$ (mL)	Volume of Deionized Water (mL)
2.00	5.00	5.00
3.00	4.00	5.00
4.00	3.00	5.00
5.00	2.00	5.00
6.00	1.00	5.00

Table 1: Spectrophotometer Standardization Samples

Next, prepare a 45 mL solution in a beaker using 3 mL of $Fe(NO_3)_3$ (0.025 M), 3 mL of $KSCN$ (0.025 M), and 39 mL of DI water. Pipette this solution into 7 separate cuvettes. Place the cuvettes in a 300 mL water bath inside glass beaker.

Setup and calibrate spectrophotometer using blank sample before running the experiment, so heat dissipated from the sample is minimized. Plug Vernier Temperature Probe into the laptop via the GoLink to log the temperature readings. Open up Logger Pro software to get live temperature readings.

Place the beaker on the hot plate and turn on the heating. Perform the following steps for 10 different temperature levels starting at 25 degrees and increasing by 5 degrees. First, use the temperature probe to determine when the sample is at the desired temperature. Wait approximately 2-3 minutes to ensure cuvettes reach same temperature as hot water bath. Pick up one cuvette using forceps and wipe off any surface water with Kimwipes. Measure the transmittance using the spectrophotometer to determine the unknown equilibrium concentrations and thus the K_c . Return the cuvette back to water bath and select another cuvette for a total of 14 trials. Repeat this whole process for the remaining temperature levels.

7 Safety, Environmental, and Ethical Concerns

Throughout this investigation, all safety, environmental, and ethical concerns were recognized and thoroughly addressed. First, the major hazard in this lab is the heating source. Thus, multiple solutions were implemented to mitigate risks. The experiment was approved and performed under teacher supervision using proper experiment apparatus such as wire gauze and beaker tongs. The glass beaker was also cooled slowly to ensure that it would not shatter upon a rapid temperature change. All these measures greatly improved safety, leading to no injuries during the course of the experiment. Second, the thiocyanatoiron(III) complex reaction utilized is relatively harmless. Still, since $Fe(NO_3)_3$ is a body tissue irritant and $KSCN$ is harmful if swallowed, in contact with skin, or inhaled, I conducted the experiment wearing safety glasses and nitrile gloves in an environment with open circulation. Third, there were no environmental concerns as a significant amount of natural resources were not utilized and pollution was not generated. Finally, there were no ethical concerns as no humans, animals, or other beings were physically or emotionally harmed in this experiment.

8 Data Collection

8.1 Quantitative Raw Data

0.1M $Fe(NO_3)_3$ (± 0.05 mL)	0.001M $KSCN$ (± 0.05 mL)	Deionized Water (± 0.05 mL)	Transmittance (± 0.00035)
2.00	5.00	5.00	0.1559
3.00	4.00	5.00	0.1992
4.00	3.00	5.00	0.2542
5.00	2.00	5.00	0.3247
6.00	1.00	5.00	0.4060

Table 2: Transmittance of Spectrophotometer Standardization Samples

T ($\pm 1^\circ C$)	Transmittance (± 0.00035)													
	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	Trial 6	Trial 7	Trial 8	Trial 9	Trial 10	Trial 11	Trial 12	Trial 13	Trial 14
25.0	0.1165	0.1172	0.1214	0.1214	0.1148	0.1144	0.1217	0.1158	0.1165	0.1172	0.1176	0.1137	0.1155	0.1190
30.0	0.1445	0.1486	0.1462	0.1406	0.1469	0.1472	0.1458	0.1486	0.1481	0.1451	0.1413	0.1472	0.1444	0.1462
35.0	0.1625	0.1716	0.1702	0.1636	0.1706	0.1647	0.1631	0.1700	0.1695	0.1625	0.1713	0.1695	0.1632	0.1643
40.0	0.1856	0.1852	0.1882	0.1964	0.1974	0.1898	0.1870	0.1831	0.1877	0.1957	0.1887	0.1880	0.1845	0.1818
45.0	0.2076	0.2051	0.2048	0.2094	0.2110	0.2093	0.2138	0.2076	0.2131	0.2142	0.2131	0.2086	0.2138	0.2131
50.0	0.2452	0.2435	0.2327	0.2354	0.2406	0.2383	0.2456	0.2407	0.2473	0.2442	0.2445	0.2463	0.2475	0.2445
55.0	0.2655	0.2648	0.2613	0.2682	0.2665	0.2773	0.2665	0.2648	0.2735	0.2717	0.2784	0.2648	0.2630	0.2717
60.0	0.3031	0.2954	0.2920	0.2829	0.2811	0.2909	0.2871	0.2902	0.2881	0.2881	0.2894	0.2784	0.2825	0.2834
65.0	0.3216	0.3129	0.3007	0.3202	0.3059	0.3087	0.3035	0.3157	0.3048	0.3185	0.3209	0.3031	0.3063	0.3077
70.0	0.3471	0.3645	0.3561	0.3414	0.3430	0.3464	0.3635	0.3625	0.3557	0.3669	0.3544	0.3408	0.3458	0.3582

Table 3: Spectrophotometer Transmittance at Various Temperatures for a Given Solution of Fe^{3+} and SCN^-

8.2 Qualitative Observations

When mixing the 0.1 M solutions, the blood red color of the solution was far too dark. Initially, my solutions seemed to get darker with temperature, which is the opposite of the expected effect. I had to dilute the solution down to millimolars in order to achieve absorbances below 1. The color of the solutions were all pale orange to pale yellow. All solutions were clear. In the middle of one of my trials, the colorimeter values dramatically changed and I realized that this was likely a failure of the colorimeter electronics. I had to redo my measurements with a new colorimeter, since the absorbance values were far different than before.

9 Analysis

9.1 Spectrophotometer Standardization

According to the Beer-Lambert Law described in Equation 2, absorbance and concentration should follow a linear trend when $0.05 < A < 1$. By creating solutions where Fe^{3+} is 100 times more abundant than SCN^- , it is safe to assume that the SCN^- is entirely reacted to form the thiocyanatoiron complex (Table 4). Thus, the precise linear trend between absorbance and concentration can be determined using these standard concentration samples. Sample calculations for the first standardization sample are shown below.

$$\text{mol } Fe^{3+} = [Fe^{3+}]_{stock} \times V_{Fe^{3+}} = 1.00 \text{ M} \times 2.00 \text{ mL} \times \frac{1 \text{ L}}{1000 \text{ mL}} = 2.00 \times 10^{-4} \text{ mol} \quad (3)$$

$$\text{mol } SCN^{-} = [SCN^{-}]_{stock} \times V_{SCN^{-}} = 0.001 \text{ M} \times 5.00 \text{ mL} \times \frac{1 \text{ L}}{1000 \text{ mL}} = 5.00 \times 10^{-6} \text{ mol} \quad (4)$$

$$[FeSCN^{2+}] = \frac{\text{mol } SCN^{-}}{V_{total}} = \frac{2.00 \times 10^{-6} \text{ mol}}{12 \text{ mL}} \times \frac{1000 \text{ mL}}{1 \text{ L}} = 4.17 \times 10^{-4} \text{ M} \quad (5)$$

	Fe^{3+}	SCN^{-}	$FeSCN^{2+}$
I	2.00×10^{-4}	5.00×10^{-6}	0
C	-5.00×10^{-6}	-5.00×10^{-6}	$+5.00 \times 10^{-6}$
E	1.95×10^{-4}	0	5.00×10^{-6}

Table 4: Moles ICE for First Spectrophotometer Standardization Sample

Equation 6 is the formula to calculate the percent uncertainty of the standardization concentrations. The conversion factors and concentration of the solutions are assumed to have negligible uncertainty.

$$\frac{\delta[FeSCN^{2+}]}{[FeSCN^{2+}]} = \frac{\delta V_{SCN^{-}}}{V_{SCN^{-}}} + \frac{\delta V_{total}}{V_{total}} = \frac{0.05 \text{ mL}}{5.00 \text{ mL}} + \frac{0.1 \text{ mL} + 0.1 \text{ mL} + 0.1 \text{ mL}}{12 \text{ mL}} = 2\% \quad (6)$$

Equation 7 calculates the absorbance A from the transmittance T . Note that absorbance has dimensionless Absorbance Units (AU). Sample calculations for the first standardization sample are shown below.

$$A = \log_{10} \frac{1}{T} = \log_{10} \frac{1}{0.1559} = 0.8172 \text{ AU} \quad (7)$$

The uncertainty for A can be determined using the Law of Propagation of Uncertainty (Taylor, 1982).

$$\delta f(x, y, \dots) = \sqrt{\left(\frac{\partial f}{\partial x} \delta x\right)^2 + \left(\frac{\partial f}{\partial y} \delta y\right)^2 + \dots} \quad (8)$$

Thus, for $A = \log_{10} \frac{1}{T}$,

$$\delta A = \delta \log_{10} \frac{1}{T} = \sqrt{\left(\frac{\partial \log_{10} \frac{1}{T}}{\partial T} \delta T\right)^2} = \frac{\delta T}{T \ln 10} = \frac{0.00035}{0.1559 \ln 10} = 0.0010 \text{ AU} \quad (9)$$

Repeating the above steps for each of the standardization samples results in Table 5 and Figure 1.

Concentration (M)	Concentration Percent Uncertainty (%)	Absorbance (AU)	Absorbance Uncertainty (AU)
4.17×10^{-4}	2	0.8172	0.0010
3.33×10^{-4}	3	0.7007	0.0008
2.50×10^{-4}	3	0.5948	0.0006
1.67×10^{-4}	4	0.4985	0.0005
8.33×10^{-5}	6	0.3915	0.0004

Table 5: Absorbance vs Standard Concentrations

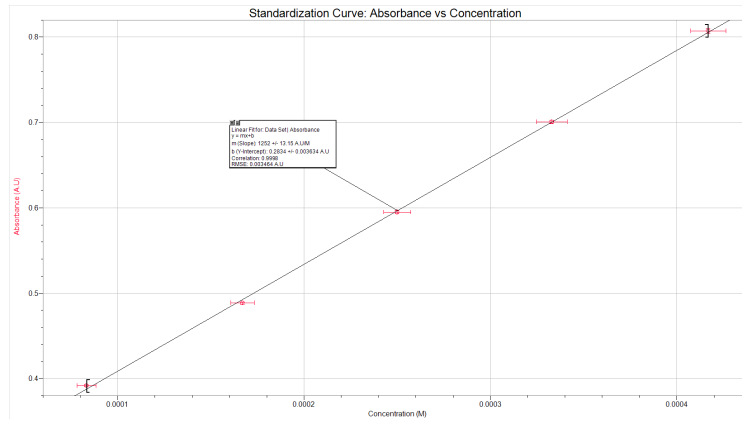


Figure 1: Standardization Curve: Absorbance vs Concentration

9.2 Relationship between Equilibrium Constant and Temperature

To determine the relationship between the equilibrium constant and the temperature, I must derive the temperature and equilibrium constant. First, when dealing with temperature, it is important to ensure that the temperature is in Kelvin, so the zero point represents absolute zero. Therefore, the following formula must be applied. During the experiment, I noticed that the temperature was often $\pm 1K$ of the true level temperature. Thus, rather than taking the uncertainty of the temperature sensor ($\pm 0.1K$), I decided to take $\pm 1K$ as the absolute uncertainty.

$$T_K = T_C + 273 = 25^\circ C + 273 = 298 K \quad (10)$$

To derive the equilibrium constant, I first calculated the initial concentrations of Fe^{3+} and SCN^- . A sample calculation is shown below.

$$[Fe^{3+}]_{init} = [Fe^{3+}]_{stock} \times V_{Fe^{3+}} = 0.0250 M \times 3.00 mL \times \frac{1}{45.0 mL} \quad (11)$$

$$= 1.67 \times 10^{-3} M \quad (12)$$

$$[SCN^-]_{init} = [SCN^-]_{stock} \times V_{SCN^-} = 0.0250 M \times 3.00 mL \times \frac{1}{45.0 mL} \quad (13)$$

$$= 1.67 \times 10^{-3} M \quad (14)$$

Next, using Equation 7, the absorbance can be derived from the transmittance. In Section 9.1, the slope of Beer-Lambert Law curve was determined to be $m = 1252.26 \pm 13.15 M^{-1}$ and the intercept was determined to be $b = 0.2835 \pm 0.0036 AU$. Thus, the concentration of $FeSCN^{2+}$ is:

$$[FeSCN^{2+}]_{eq} = \frac{A - b}{m} = \frac{0.9337 AU - 0.2835 AU}{1252.26 M^{-1}} = 5.192 \times 10^{-4} M \quad (15)$$

	Fe^{3+}	SCN^-	$FeSCN^{2+}$
I	1.67×10^{-3}	1.67×10^{-3}	0
C	$-x$	$-x$	$+x$
E	$(1.67 \times 10^{-3}) - x$	$(1.67 \times 10^{-3}) - x$	x

Table 6: Concentration ICE for Given $[FeSCN^{2+}]_{eq}$

The equilibrium constant can be calculated using the following formula. Table 6 can be used to reduce the formula further.

$$K_c = \frac{[FeSCN^{2+}]_{eq}}{[Fe^{3+}]_{eq}[SCN^-]_{eq}} \quad (16)$$

$$= \frac{[FeSCN^{2+}]_{eq}}{([Fe^{3+}]_{init} - [FeSCN^{2+}]_{eq}) \times ([SCN^-]_{init} - [FeSCN^{2+}]_{eq})} \quad (17)$$

$$= \frac{5.192 \times 10^{-4} M}{(1.67 \times 10^{-3} M - 5.192 \times 10^{-4} M) \times (1.67 \times 10^{-3} M - 5.192 \times 10^{-4} M)} \quad (18)$$

$$= 394 \quad (19)$$

The percent uncertainty of K_c can be estimated using the following formula. The conversion factors and concentration of the solutions are assumed to have negligible uncertainty.

$$\frac{\delta[Fe^{3+}]_{init}}{[Fe^{3+}]_{init}} = \frac{0.05 mL}{3.00 mL} + \frac{0.2 mL}{45.0 mL} = 2\% \quad (20)$$

$$\frac{\delta[SCN^-]_{init}}{[SCN^-]_{init}} = \frac{0.05 mL}{3.00 mL} + \frac{0.2 mL}{45.0 mL} = 2\% \quad (21)$$

$$\frac{\delta[FeSCN^{2+}]_{eq}}{[FeSCN^{2+}]_{eq}} = \frac{0.0013 AU + 0.0036 AU}{0.6502 AU} + \frac{13.15 M^{-1}}{1252.26 M^{-1}} = 1.8\% \quad (22)$$

$$\frac{\delta K_c}{K_c} = \frac{\delta[FeSCN^{2+}]_{eq}}{[FeSCN^{2+}]_{eq}} + \frac{\delta[Fe^{3+}]_{eq}}{[Fe^{3+}]_{eq}} + \frac{\delta[SCN^-]_{eq}}{[SCN^-]_{eq}} \quad (23)$$

$$= 1.8\% + \frac{4 \times 10^{-5} M}{1.15 \times 10^{-3} M} + \frac{4 \times 10^{-5} M}{1.15 \times 10^{-3} M} \quad (24)$$

$$= 10\% \quad (25)$$

I repeated the above steps for each of the trials and levels in Table 3 to create Table 7. Figure 2 is a plot of the equilibrium constant vs temperature data for the first trial. Similar results were found in the other trials.

Temperature ($\pm 1K$)	Equilibrium Constant													
	Trial 1	Trial 1 Percent Uncertainty (%)	Trial 2	Trial 2 Percent Uncertainty (%)	Trial 3	Trial 3 Percent Uncertainty (%)	Trial 4	Trial 4 Percent Uncertainty (%)	Trial 5	Trial 5 Percent Uncertainty (%)	Trial 6	Trial 6 Percent Uncertainty (%)	Trial 7	Trial 7 Percent Uncertainty (%)
298	394	10	391	10	374	10	374	10	402	10	404	10	373	10
303	298	10	287	10	293	10	309	10	291	10	290	10	294	10
308	253	10	234	10	237	10	251	10	236	10	248	10	252	10
313	209	9	209	9	204	9	192	9	190	9	202	9	206	9
318	176	9	179	9	179	9	173	9	171	9	173	9	167	9
323	132	9	134	9	145	9	142	9	137	9	139	9	132	9
328	114	9	114	9	117	9	111	9	113	9	104	9	113	9
333	85.8	9	90.9	9	93.3	9	99.9	9	101	9	94.1	9	96.8	9
338	74.3	9	79.5	9	87.3	9	75.1	9	83.9	9	82.2	9	85.5	9
343	60.4	9	51.9	10	55.9	10	63.3	9	62.5	9	60.7	9	52.4	10

Equilibrium Constant (Continued.)													
Trial 8	Trial 8 Percent Uncertainty (%)	Trial 9	Trial 9 Percent Uncertainty (%)	Trial 10	Trial 10 Percent Uncertainty (%)	Trial 11	Trial 11 Percent Uncertainty (%)	Trial 12	Trial 12 Percent Uncertainty (%)	Trial 13	Trial 13 Percent Uncertainty (%)	Trial 14	Trial 14 Percent Uncertainty (%)
397	10	394	10	391	10	390	10	407	10	399	10	384	10
287	10	288	10	296	10	307	10	290	10	298	10	293	10
237	10	238	10	253	10	235	10	238	10	252	10	249	10
213	9	205	9	193	9	204	9	205	9	211	9	215	9
176	9	168	9	167	9	168	9	174	9	167	9	168	9
137	9	130	9	133	9	133	9	131	9	130	9	133	9
114	9	107	9	109	9	103	9	114	9	116	9	109	9
94.6	9	96.1	9	96.1	9	95.1	9	103	9	100	9	99.5	9
77.8	9	84.7	9	76.1	9	74.7	9	85.8	9	83.7	9	82.8	9
52.9	10	56.1	10	50.8	10	56.7	10	63.6	9	61	9	54.9	10

Table 7: Equilibrium Constant vs Temperature

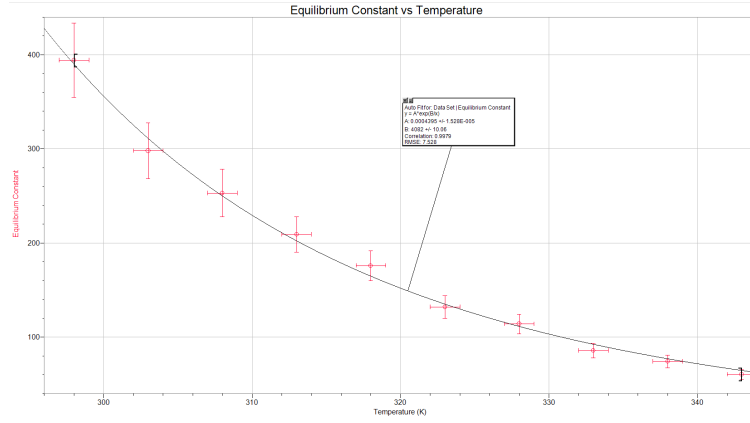


Figure 2: Graph of Equilibrium Constant vs Temperature

9.3 Linearization

As seen in Figure 2, there is a very strong correlation ($R^2 = 0.9979$) to a $K_c(T) = Ae^{B/T}$ curve, where A and B are coefficients. This matches the expected linearization as shown below.

Setting the equations $\Delta G^\circ = -RT \ln K_c$ and $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$ equal to each other.

$$-RT \ln K_c = \Delta H^\circ - T\Delta S^\circ \quad (26)$$

$$\ln K_c = -\frac{\Delta H^\circ}{R} \times \frac{1}{T} + \frac{\Delta S^\circ}{R} \quad (27)$$

Equation 27 indicates that by taking the natural log of K_c and the reciprocal of temperature the relationship should be linear. A sample calculation is shown for this linearization.

$$\text{Reciprocal of Temperature} = \frac{1}{T_K} = \frac{1}{298 \text{ K}} = 0.00336 \text{ K}^{-1} \quad (28)$$

The uncertainty of $\frac{1}{T_K}$ can be determined using Equation 8,

$$\delta \left(\frac{1}{T_K} \right) = \sqrt{\left(\frac{\partial \left(\frac{1}{T_K} \right)}{\partial T_K} \delta T_K \right)^2} = \frac{\delta T_K}{T^2} = \frac{1 \text{ K}}{(298 \text{ K})^2} = 1 \times 10^{-5} \text{ K}^{-1} \quad (29)$$

$$\frac{\delta \left(\frac{1}{T_K} \right)}{\frac{1}{T_K}} = 0.34\% \quad (30)$$

Similarly,

$$\text{Natural Log of Equilibrium Constant} = \ln K_c = \ln 394 = 5.98 \quad (31)$$

$$\delta \ln K_c = \sqrt{\left(\frac{\partial \ln K_c}{\partial T} \delta T \right)^2} = \frac{\delta K_c}{K_c} = \frac{37.59}{394} = 0.10 \quad (32)$$

$$\frac{\delta \ln K_c}{\ln K_c} = 1.8\% \quad (33)$$

Repeating the above steps for each of the measurements to create Table 8.

Reciprocal of Temperature (1/K)	Reciprocal of Temperature Percent Uncertainty (%)	Natural Log of Equilibrium Constant											
		Trial 1	Trial 1 Percent Uncertainty (%)	Trial 2	Trial 2 Percent Uncertainty (%)	Trial 3	Trial 3 Percent Uncertainty (%)	Trial 4	Trial 4 Percent Uncertainty (%)	Trial 5	Trial 5 Percent Uncertainty (%)	Trial 6	Trial 6 Percent Uncertainty (%)
0.00336	0.34	5.98	1.8	5.97	1.8	5.92	1.7	5.92	1.7	6.00	1.8	6.00	1.8
0.00330	0.33	5.70	1.7	5.66	1.7	5.68	1.7	5.73	1.7	5.67	1.7	5.67	1.7
0.00325	0.32	5.53	1.7	5.46	1.8	5.47	1.8	5.52	1.7	5.46	1.8	5.52	1.7
0.00320	0.32	5.34	1.8	5.34	1.8	5.32	1.8	5.26	1.8	5.25	1.8	5.31	1.8
0.00315	0.31	5.17	1.8	5.19	1.8	5.19	1.8	5.15	1.8	5.14	1.8	5.15	1.8
0.00310	0.31	4.88	1.9	4.90	1.9	4.98	1.8	4.96	1.8	4.92	1.9	4.94	1.9
0.00305	0.30	4.73	1.9	4.74	1.9	4.76	1.9	4.71	1.9	4.73	1.9	4.65	2.0
0.00300	0.30	4.45	2.0	4.51	2.0	4.54	2.0	4.60	2.0	4.62	2.0	4.54	2.0
0.00296	0.30	4.31	2.0	4.38	2.0	4.47	2.0	4.32	2.0	4.43	2.0	4.41	2.0
0.00292	0.29	4.10	2.0	3.95	2.0	4.02	2.0	4.15	2.0	4.13	2.0	4.11	2.0

Natural Log of Equilibrium Constant (Continued.)															
Trial 7	Trial 7 Percent Uncertainty (%)	Trial 8	Trial 8 Percent Uncertainty (%)	Trial 9	Trial 9 Percent Uncertainty (%)	Trial 10	Trial 10 Percent Uncertainty (%)	Trial 11	Trial 11 Percent Uncertainty (%)	Trial 12	Trial 12 Percent Uncertainty (%)	Trial 13	Trial 13 Percent Uncertainty (%)	Trial 14	Trial 14 Percent Uncertainty (%)
5.92	1.7	5.98	1.8	5.98	1.8	5.97	1.8	5.97	1.8	6.01	1.8	5.99	1.8	5.95	1.7
5.68	1.7	5.66	1.7	5.66	1.7	5.69	1.7	5.73	1.7	5.67	1.7	5.70	1.7	5.68	1.7
5.53	1.7	5.47	1.8	5.47	1.8	5.53	1.7	5.46	1.8	5.47	1.8	5.53	1.7	5.52	1.7
5.33	1.8	5.36	1.8	5.32	1.8	5.26	1.8	5.32	1.8	5.32	1.8	5.35	1.8	5.37	1.8
5.12	1.8	5.17	1.8	5.13	1.8	5.12	1.8	5.13	1.8	5.16	1.8	5.12	1.8	5.13	1.8
4.88	1.9	4.92	1.9	4.87	1.9	4.89	1.9	4.89	1.9	4.88	1.9	4.87	1.9	4.89	1.9
4.73	1.9	4.74	1.9	4.67	1.9	4.69	1.9	4.64	2.0	4.74	1.9	4.75	1.9	4.69	1.9
4.57	2.0	4.55	2.0	4.57	2.0	4.57	2.0	4.56	2.0	4.64	2.0	4.61	2.0	4.60	2.0
4.45	2.0	4.35	2.0	4.44	2.0	4.33	2.0	4.31	2.0	4.45	2.0	4.43	2.0	4.42	2.0
3.96	2.0	3.97	2.0	4.03	2.0	3.93	2.0	4.04	2.0	4.15	2.0	4.11	2.0	4.01	2.0

Table 8: Natural Log of Equilibrium Constant vs Reciprocal of Temperature

Finally, the average natural log of the equilibrium constant was determined for each of the reciprocal of temperature levels. The uncertainty of this average can be determined using the following formula. A sample calculation is shown below.

$$\delta(\ln K_c)_{avg} = \frac{(\ln K_c)_{max} - (\ln K_c)_{min}}{2\sqrt{N}} = \frac{6.01 - 5.92}{2\sqrt{14}} = 0.01 \quad (34)$$

$$\frac{\delta(\ln K_c)_{avg}}{(\ln K_c)_{avg}} = 0.19\% \quad (35)$$

Performing the average calculation for each reciprocal of temperature level, I created Table 9 and Figure 3.

Reciprocal of Temperature (1/K)	Reciprocal of Temperature Percent Uncertainty (%)	Average Natural Log of Equilibrium Constant	Average Natural Log of Equilibrium Constant Percent Uncertainty (%)
0.00336	0.34	5.97	0.19
0.00330	0.33	5.68	0.18
0.00325	0.32	5.50	0.19
0.00320	0.32	5.32	0.31
0.00315	0.31	5.15	0.17
0.00310	0.31	4.90	0.30
0.00305	0.30	4.71	0.36
0.00300	0.30	4.57	0.55
0.00296	0.30	4.39	0.49
0.00292	0.29	4.05	0.73

Table 9: Average Natural Log of Equilibrium Constant vs Reciprocal of Temperature

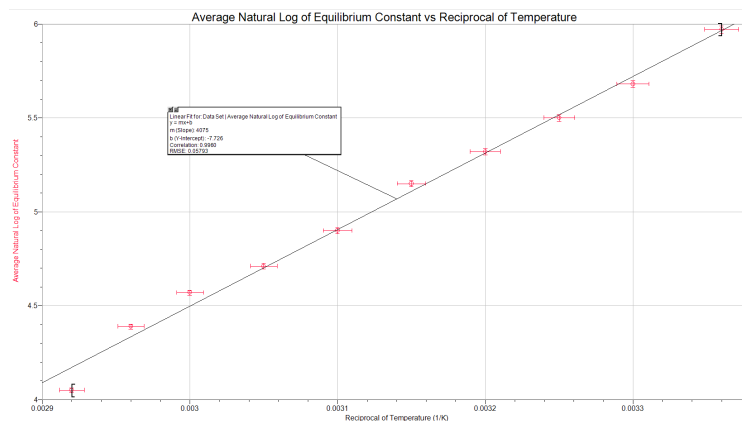


Figure 3: Graph of Average Natural Log of Equilibrium Constant vs Reciprocal of Temperature

9.4 Interpretation

As seen in Figure 3), the line of best fit indicates a positive linear relationship between $\ln K_c$ and $\frac{1}{T}$. This means as $\frac{1}{T}$ increases, $\ln K_c$ will increase proportionally. Thus, this linearization proves that there is a negative exponential relationship between K_c and T .

There is a very strong correlation ($R^2 = 0.9960$) between the linear regression and the linearized data. The line of best fit passes through almost all points and uncertainty bars. The minimum and maximum slope lines are very similar to the regression line. All this affirms that the K_c and T of a thiocynatoiron complex reaction follow a negative exponential relationship.

Finally, the slope and intercept of this linearized graph is proportional to the standard enthalpy change and entropy change of the reaction respectively, as shown in Equation 27. Thus, the formation of the thiocynatoiron complex is exothermic and decreases entropy. The small ΔH° and ΔS° may be due to the formation of weak coordinate covalent bonds in the thiocyanatoiron complex.

$$\Delta H^\circ = -m \times R = -4075 \text{ K} \times 8.314 \text{ J mol}^{-1} \text{ K}^{-1} = -33880 \text{ J mol}^{-1} \quad (36)$$

$$\Delta S^\circ = b \times R = -7.726 \times 8.314 \text{ J mol}^{-1} \text{ K}^{-1} = -64.23 \text{ J mol}^{-1} \text{ K}^{-1} \quad (37)$$

10 Conclusion

Therefore, according to this experiment, there is a very strong correlation ($R^2 = 0.9960$) for a negative exponential relationship between the equilibrium constant and the temperature of a thiocyanatoiron complex reaction. This matches my hypothesis for this experiment. Furthermore, the individual trial percent uncertainties was far below 5%, which means that my measurement system is precise. The average percent uncertainties were also far below 5% which means that the experiment had a precise procedure. Finally, the derived enthalpy and entropy change was well within the accepted range, suggesting fairly accurate results throughout.

11 Sources for Error

Error could have been introduced from 4 sources: measurement of temperature using the Vernier Temperature Probe, measurement of transmittance using the spectrophotometer, the indirect heating of the cuvettes using a water bath, and temperature variations during the procedure.

First, the measurement of temperature using the Vernier Temperature Probe contributes to random error since the device uncertainty for the probe is $\pm 0.1 \text{ K}$. The random error from this source

is negligible in this experiment. Next, the measurement of transmittance using the spectrophotometer also contributes to random error since the device uncertainty for the device is ± 0.00035 . The random error from this source is also negligible in this experiment. Then, since the cuvettes were indirectly heated through a water bath, the temperature of the water could have been higher than that of the cuvettes leading to systematic error. However, since the heating was put on the lowest setting and the temperature of the cuvettes and the heat bath was normalized by waiting 2-3 minutes, the temperature of the cuvettes should have been relatively close to the temperature of the water bath. Hence, the systematic error from this source is negligible. Finally, as I removed the cuvettes from the hot water bath, wiped off the water on the surface, and placed the sample in the spectrophotometer, the temperature of the small sample likely changed fairly dramatically. This would contribute to a significant systematic error. To account for this, I increased my temperature uncertainty to $\pm 1\text{ K}$.

In conclusion, most sources of error were minimal or well-accounted for throughout the experiment.

12 Strengths

One strength of this experiment is the use of the spectrophotometer to measure the concentration of the colored $FeSCN^{2+}$ complex. Other methods to measure the concentration like titration would have taken much longer to complete. Since the spectrophotometer could measure the concentration in a few seconds, minimal temperature was lost from the cuvettes. Furthermore, the ability to take fast measurements enabled me to take a large number of trials and temperature levels. Thus, the use of the spectrophotometer significantly improved the accuracy and precision of this experiment. Another major strength of this experiment was the use of multiple cuvettes in the hot water bath. This allowed me to take all the transmittance measurements for a temperature level at the same time, greatly improving the speed of the experiment. Furthermore, when cuvettes were removed from the water bath, they would decrease in temperature slightly. However, by cycling through the cuvettes, each cuvette has enough time to return to the temperature of the hot water bath.

13 Weaknesses

One weakness of this experiment was the drop in temperature of the cuvettes, while the measurement was taken. Though the measurement time was limited, the drop in temperature was still significant. Another weakness of this experiment was maintaining a consistent temperature for the water bath. Though the hot plate held the temperature relatively constant, it deviated by $\pm 1^\circ C$, significantly increasing the random error and thus the percent uncertainty in the temperature. These were major experiment design flaws that need to be revised for future trials.

14 Improvements

Multiple improvements could be applied to this experiment to address its weaknesses. First, the use of cuvettes made of a more thermally insulating material could reduce the magnitude of the temperature drop. Furthermore, a correction factor could also be developed to adjust the measurements for the impact of temperature drop. Second, the volume of the water bath could be increased. Though it would take a longer period to heat the bath, it would also take a longer pe-

riod for the bath to cool down. This would greatly diminish the random error from the fluctuating temperature and thus decrease the temperature percent uncertainty. These improvements would greatly improve both the accuracy and precision of this experiment.

15 Extensions

A possible extension to this experiment that might be worthy of future study is the relationship between the equilibrium constant and pressure. This experiment explored the relationship between the equilibrium constant and temperature as described by the Van 't Hoff Equation. However, in industrial processes, temperature is modulated along with pressure to achieve ideal operating conditions. Thus, understanding the precise relationship between the equilibrium constant and pressure is significant.

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