



*Note: Data was obtained from Thomas Anglais 8298567*

## **Introduction**

In the study of molecular kinetics, the rate of a reaction can be determined experimentally by using the reactant's absorbance of light. This is particularly useful when other methods of determining the concentration of reactant or product are not available or would interfere too much with the experiment. The data was obtained using a SpectroVis and was recorded using a LabQuest 2. The theory behind this experiment is the study of the order of a reaction, which can be understood as a reactions dependency on the concentration of the reactant(s), product(s), or a combination of both. The rate of a reaction can also be affected by the presence of heat, light, or change in conditions including acidity, basicity, and solvent choice. In our experiment we altered the acidity of the reaction by a factor of 0.5 in three separate trials. However, this was shown to have no affect on the reaction, given the limitations of the experiment. Reactions are typically first or second order. In first order kinetics, the rate of the reaction depends on the concentration of a single reactant and as the amount of this reactant increases, the rate,  $k$ , increases. In second order kinetics, the rate depends on the concentration of two reactants, or depends doubly on a single reactant. Pseudo-first order kinetics is a combination of the two, in which a second order reaction is manipulated so as to produce the results of a first order reaction<sup>1</sup>. This is possible by limiting the quantity of one of the reactants, and in this case, the chromium was limited to several drops while the EDTA was left in large amounts. The effect this has on the experiment is one reactant is in such small proportions that it has negligible effects on the rate of the reaction, and so the reaction is roughly first order in terms of the reactant in the higher quantity. A major goal of our experiment was to determine if this reaction exhibited pseudo-first order kinetics. This was achieved using experimental data and by deriving the rate equation in order to plot several different graphs.

## **Procedure**

*As outlined in the CHM1301 lab manual for Experiment 3: Chemical Kinetics.*

## **Observations**

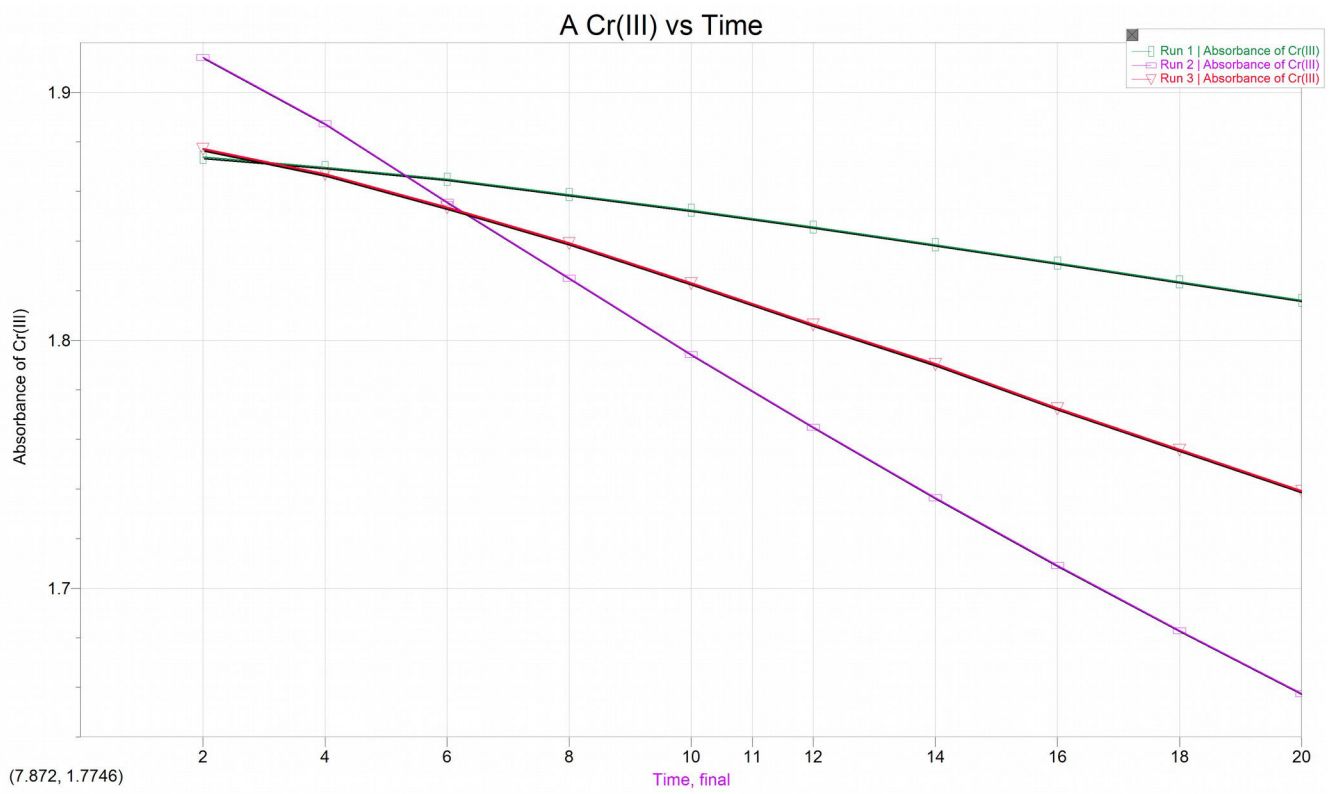
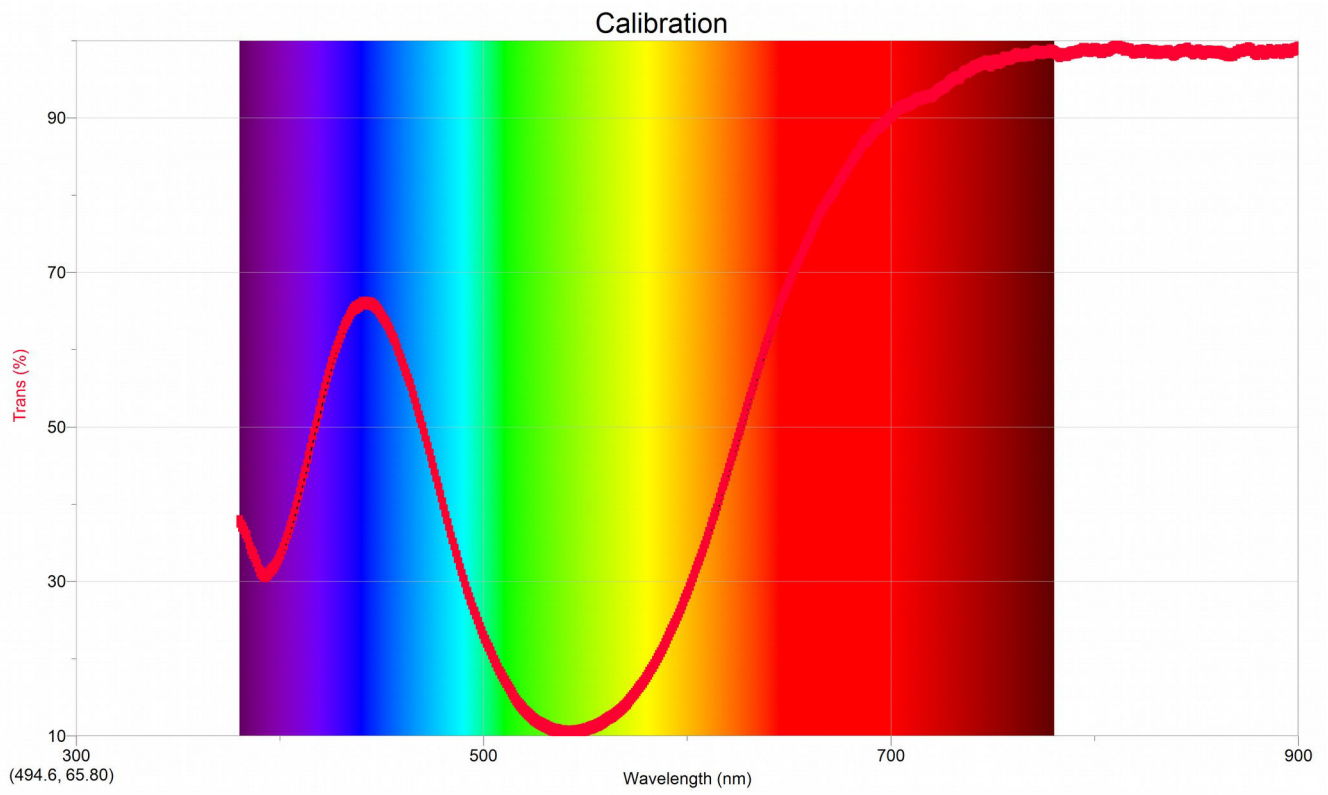
-Colour changed to deep purple when Cr (III) was added to EDTA

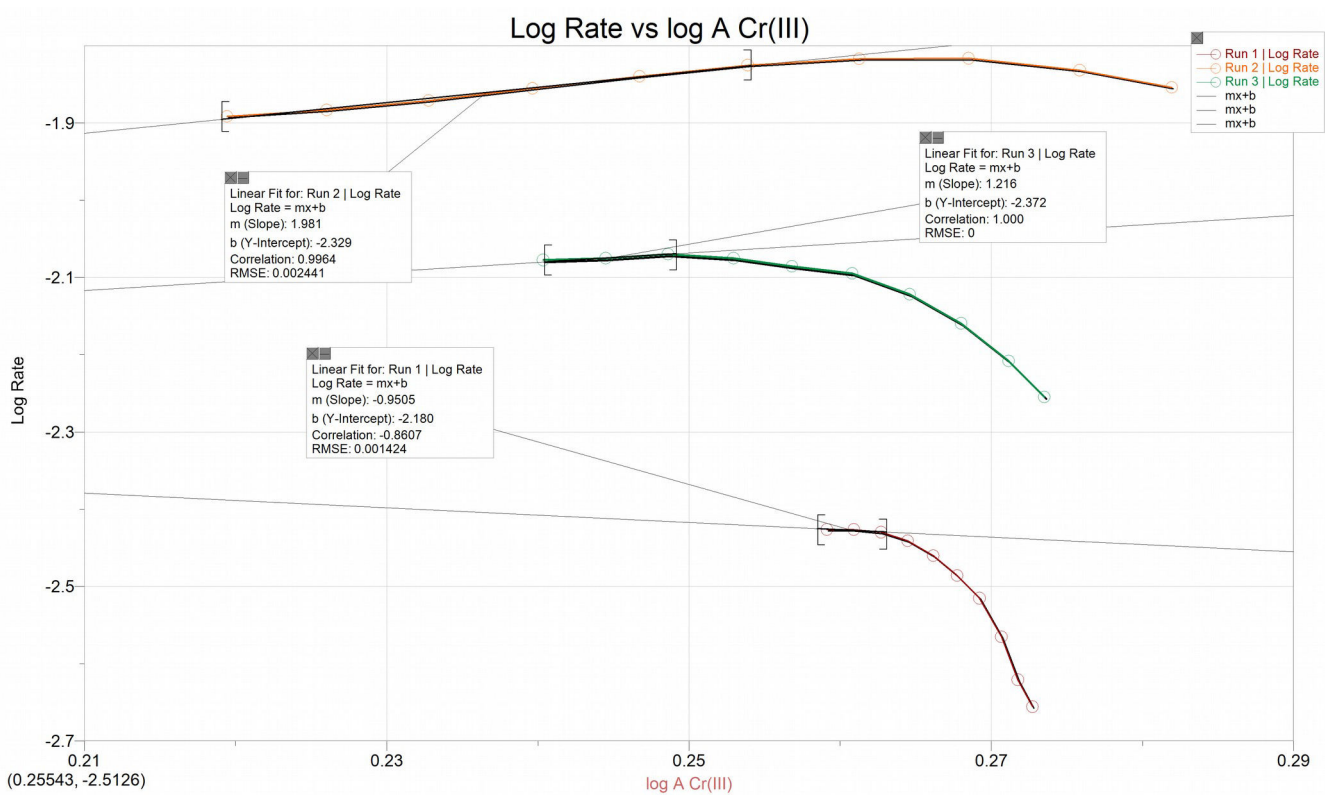
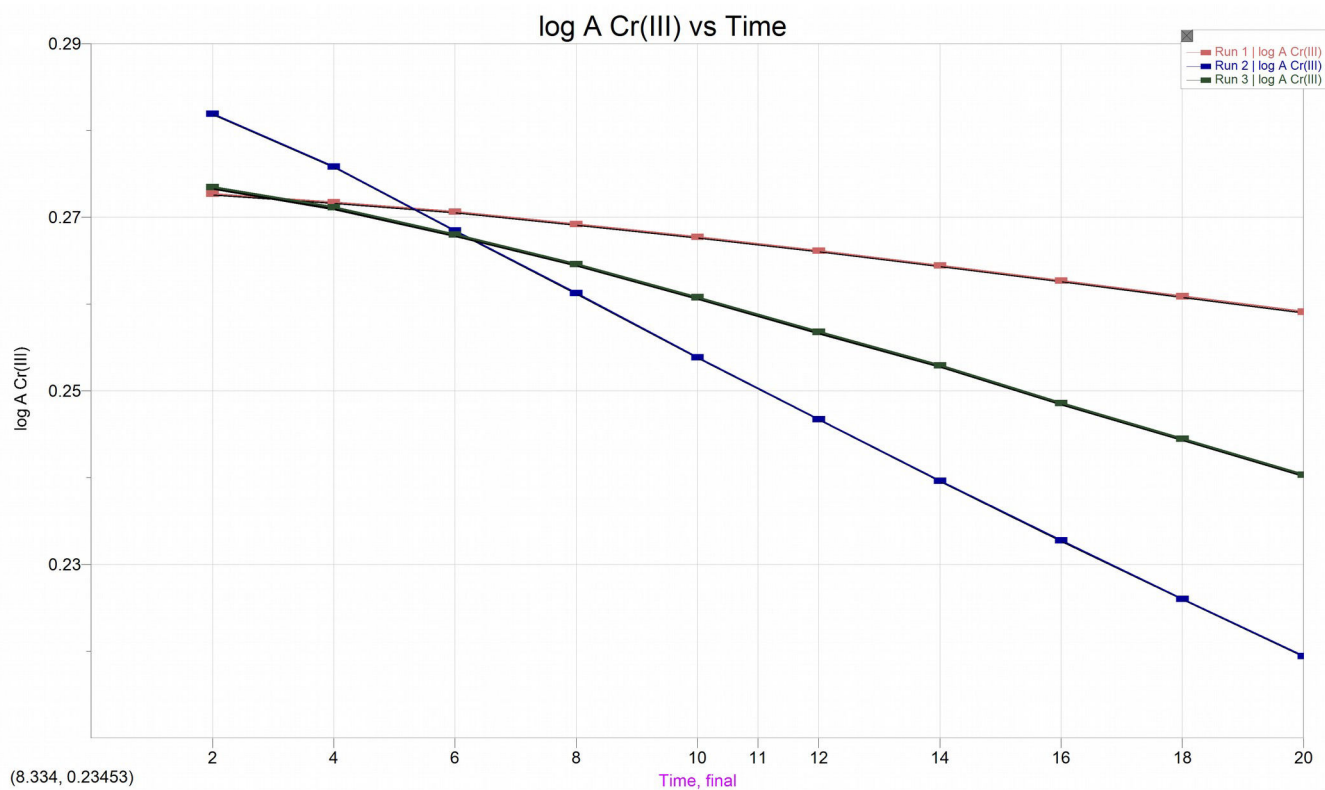
## **Results**

### **Graphs**

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<sup>1</sup> [http://chemwiki.ucdavis.edu/Physical\\_Chemistry/Kinetics/Reaction\\_Rates/Second-Order\\_Reactions/Pseudo-1st-order\\_reactions](http://chemwiki.ucdavis.edu/Physical_Chemistry/Kinetics/Reaction_Rates/Second-Order_Reactions/Pseudo-1st-order_reactions)





### Sample calculations

At pH 5.0 and time 4, A Cr was calculated as follows:

$$\begin{aligned} A \text{ Cr (III)} &= A(\infty) - A(t) \\ &= 1.9522 - 0.098606 \\ &= 1.854 \end{aligned}$$

At pH 5.0 and time 4, log A Cr (III) was calculated as follows:

$$\begin{aligned} \log A \text{ Cr (III)} \\ &= \log 1.839 \\ &= 0.265 \end{aligned}$$

At pH 5.0 and time 4, rate was calculated as follows:

$$\begin{aligned} \text{Rate} &= -\text{derivative}(A \text{ Cr(III)}, A(t)) \\ &= -\text{derivative}(1.839, 0.098606) \\ &= 0.00755 \end{aligned}$$

At pH 5.0 and time 4, log rate was calculated as follows:

$$\begin{aligned} \log (\text{Rate}) \\ &= \log (0.00755) \\ &= -2.122 \end{aligned}$$

At pH 5.0 and time 4, log A Cr was calculated as follows:

$$\begin{aligned} \log (A \text{ Cr}) \\ &= \log (1.839) \\ &= 0.265 \end{aligned}$$

**Table 2.** Results

pH	Time (min)	Trans @ 542 nm	A(t)	A Cr	A Cr(III)	Time,final	log A Cr(III)	Rate	Log Rate	
4	0	87.7061482207	0.0569699614	1.8762300386	1.8738419984	2	0.2727329686	0.002209116	-2.6557814854	
	2	87.2252049161	0.0593580016	1.8738419984	1.8696423181	4	0.2717585294	0.002394178	-2.6208435592	
	4	86.3857917525	0.063557682	1.8696423181	1.864960431	6	0.2706696218	0.0027214574	-2.5651984642	
	6	85.4595164279	0.068239569	1.864960431	1.8587556488	8	0.2692223014	0.0030525479	-2.5153375193	
	8	84.2472335674	0.0744443512	1.8587556488	1.8524411228	10	0.2677444134	0.003267229	-2.4858204302	
	10	83.0311633336	0.0807588772	1.8524411228	1.8457067645	12	0.2661627039	0.0034651465	-2.4602783942	
	12	81.7535771596	0.0874932355	1.8457067645	1.8385389882	14	0.264472844	0.0036223091	-2.4410144965	
	14	80.41535586	0.0946610118	1.8385389882	1.8311061208	16	0.2627135143	0.0037164754	-2.4298687411	
	16	79.0507729524	0.1020938792	1.8311061208	1.8235376757	18	0.2609147406	0.003746125	-2.4264177355	
	18	77.6850904409	0.1096623243	1.8235376757	1.8160655301	20	0.2591315154	0.0037456817	-2.426469134	
	20	76.3599314969	0.1171344699	1.8160655301						
	22	1.1594302229	1.9357553831	-0.0025553831						
	24	1.1663682947	1.9331642943	3.57E-05						
	4.5	0	88.7291030975	0.0519339084	1.9244660916	1.914011293	2	0.2819444959	0.0139972119	-1.8539584617
		2	86.6186265107	0.062388707	1.914011293	1.8873567448	4	0.2758539975	0.0147309437	-1.8317694305
		4	81.4623144543	0.0890432552	1.8873567448	1.8556725482	6	0.2685013431	0.0152657833	-1.8162809058
		6	75.7308006203	0.1207274518	1.8556725482	1.8250188309	8	0.26126735	0.0152423525	-1.8169479988
		8	70.5697909467	0.1513811691	1.8250188309	1.7942716964	10	0.2538882065	0.0149541572	-1.8252380582
		10	65.7463574286	0.1821283036	1.7942716964	1.7649476385	12	0.2467318255	0.0144640507	-1.8397100633
		12	61.4536437585	0.2114523615	1.7649476385	1.7363968972	14	0.2396490011	0.0139491575	-1.8554520233
		14	57.5435826202	0.2400031028	1.7363968972	1.7091251105	16	0.2327738549	0.0134570432	-1.8710503352
		16	54.0412157304	0.2672748895	1.7091251105	1.6828152486	18	0.2260364387	0.0130845416	-1.8832414872
		18	50.8645549195	0.2935847514	1.6828152486	1.6574515893	20	0.2194408524	0.0128399668	-1.8914360985
		20	47.9790438958	0.3189484107	1.6574515893					
22		1.0557532385	1.9764375777	-3.76E-05						
5		0	85.4765751894	0.0681528871	1.8840471129	1.8771865345	2	0.2735074303	0.0055630713	-2.2546853777
		2	84.1369054242	0.0750134655	1.8771865345	1.8670280551	4	0.271150844	0.0061920157	-2.2081679478
		4	82.1917173933	0.0851719449	1.8670280551	1.8535935561	6	0.268014511	0.0069250862	-2.1595748171
		6	79.6881154135	0.0986064439	1.8535935561	1.8391212195	8	0.2646103552	0.0075530412	-2.121878144
		8	77.0763640733	0.1130787805	1.8391212195	1.823035156	10	0.2607950438	0.0080401102	-2.0947379971
		10	74.2737165649	0.129164844	1.823035156	1.8063610767	12	0.2568045666	0.0082100596	-2.0856536918
		12	71.4761376845	0.1458389233	1.8063610767	1.7903941009	14	0.2529486383	0.0084091677	-2.0752469869
		14	68.8960147179	0.1618058991	1.7903941009	1.7725797687	16	0.2486057882	0.0085114767	-2.069995087
		16	66.127144395	0.1796202313	1.7725797687	1.7558631152	18	0.2444906559	0.0084139563	-2.0749997468
		18	63.6301746422	0.1963368848	1.7558631152	1.7392090402	20	0.2403517841	0.0083662201	-2.0774707162
		20	61.2363138369	0.2129909599	1.7392090402					
		22	1.1162660474	1.9522322847	-3.23E-05					

## Analysis

In a normal chemical reaction, the concentration of the reactant decreases while the concentration of the product increases. This lab provided a secondary method of obtaining the amount of either the product or the reactant at any given time by measuring the amount of light that was absorbed during the reaction. The experiment was attempted in three reaction conditions, which all had different pH values. Changing the pH value from 4.0 to 4.5 and performing the experiment was seen to have no effect on the outcome of the experiment. The same could be said about adjusting the pH to 5.0. This doesn't rule out the effect of pH however, as another test would need to be performed where the concentration of Chromium was held constant and the pH would be varied to compare the results of both tests and see how the rate of light absorbance was affected. In our experiment we chose to measure the data as a percentage of transmittance of light instead of a logarithmic expression. The values for the percent transmittance in each experiment were between 1-100% and therefore were plausible. Our data table shows that the value for transmittance (Trans @ 542 nm) is increasing as you go down the column, which indicates the product (EDTA-chromium complex) is increasing in its absorbance of the light, which suggests that the product is increasing in concentration. This is a reasonable result according to the theory of the experiment, and also is evidence that the reactant, Chromium, is diminishing. In our experiment we waited only 20 minutes for each reaction to take place, where the reaction should realistically take generally 4-6 hrs. to get to completion. Because we didn't do the reaction for long enough, we had to heat the reaction in boiling water to finish it off. The impact of this on the experiment is that the end results were drastically compressed, and were less accurate than if we had allowed it to proceed to the estimated completion time. However, for our purposes, we assumed that the final time, 22 minutes, represented the infinite time, A(t) infinity, where all the chromium had become

the complex. By subtracting  $A(t)$  infinity from any given time,  $A(t)$ , we were able to obtain the absorbance of chromium reactant at a specific time. In each experiment, the rate was shown to model the equation:

$$\text{rate} = k[\text{Cr}]^m[\text{EDTA}]^n[\text{H}^+]^p$$

By keeping  $[\text{EDTA}]^n[\text{H}^+]^p$  constant we observed the formula  $\text{rate} = k[\text{Cr}]^m$ , which when rearranged into the expression “ $y=mx+b$ ” gave us a value of  $m$  (slope) that described the partial order of the reaction. For the graph of experiment 1, the slope was  $-0.9505$ . A negative partial order does not make sense to the experiment, but the fact that the value was close to 1 means that it was not far from a straight line. For the graph of experiment 2, the slope was  $1.981$ . This was seen to be a closer match to a straight line, as would have been expected for a reaction with a partial order of 1. The closest value to 1 was shown for the graph of experiment 3. In this case the slope of the line was  $1.216$ . The data from this portion of the experiment shows that on average the reactions follow pseudo-first order kinetics. However, the experiment was shown to be flawed based on the curve of each graph, and one could speculate that these graphs were not straight lines due to a combination of factors. Firstly, the fact that the linear lines of best fit were drawn manually and not by a computer leaves a margin of error. As well, the experiments were performed with an expected degree of error as the measurements of EDTA and Chromium were not exact (ie. fill the cuvette 3/4 full...). Finally, in the last step where the reaction vessel was removed, heated, and returned to finish off the reaction would have a lot of variables that could influence the graph, including the length of time spent switching the vessel and the precise temperature the solution started at and ended at. Looking forwards, if the experiment were to be reproduced, the main area that we would try to improve upon would be trying to keep the length of times for boiling or transferring the reaction mixture consistent so as to be scientifically viable.

$$\begin{aligned}MM_{\text{zinc}} &= 25 \text{ J/mol} \cdot ^\circ\text{C} / (0.0365 \text{ g} \cdot ^\circ\text{C}) \\ &= 690 \text{ g/mol}\end{aligned}$$

### Lab 3

- Wavelength minimum % Trans = 8.208 @ 536.60  
which is close to 540 nm ∴ 😊

- 10 mL 4.0 pH EDTA

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