Title Page

Title (1 pts)

The NMR of My Enemy is My Friend

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Two Hypotheses (4 pts)

In general, it is believed that the magnitude of the T_1 and T_2 value plots will correlate to the amount of hydrogen atoms present. This implies that the T_1 and T_2 value plots for light mineral oil will show the steepest slopes, and will decrease in order from heavy mineral oil to water to water w/ $FeCl_3$. This is believed because NMR tends to affect only hydrogen atoms. The molecular makeup of both mineral oils consist of hydrocarbons, but heavy mineral oil tends to have more cyclic hydrocarbons, while light mineral oil tends to have more linear hydrocarbons. Cyclic hydrocarbons tend to have less hydrogens than linear carbons (for example, 12 hydrogens in cyclohexane vs 14 hydrogens in hexane). Likewise, water w/ $FeCl_3$ will remain unchanged compared to water, as $FeCl_3$ is not detected in NMR spectroscopy.

It is also believed that the samples with more hydrogen atoms will show longer T_1 and T_2 relaxation times. This is considered in thinking about how a higher density of hydrogen atoms would correspond to more magnetic moments present in the molecules and would result in a longer time for more amounts of these atoms to fully relax.

Abstract (5 pts)

This experiment was performed in order to get a greater insight into how atoms react when introduced into a magnetic field. In general, atoms tend to try and align their spin to be parallel to the magnetic field. There are many other forces, such as intermolecular interference, that can make this alignment take much longer to accomplish. Likewise, removing the samples from the magnetic field would mean that the other forces would cause the relaxation of the atomic spin to take longer.

In this experiment, four different samples were introduced to a magnetic field inside of a TeachSpin PSA-2 pulsed NMR instrument, in the hopes of determining the T_1 and T_2 relaxation values for each of the samples. In the end, it was determined that water with $FeCl_3$ had the highest T_1 relaxation time, followed by water, then followed by light mineral oil, leaving heavy mineral oil with the lowest T_1 relaxation time. For T_2, water should the longest relaxation time, followed by light mineral oil, followed then by water with $FeCl_3$, leaving heavy mineral oil with the shorter T_2 relaxation time.

Results (35 pts)

In the experimental procedure, a total of eight plots were constructed from the values received from the TeachSpin PS2-A. There are four plots for the T_1 magnetization values and four for the T_2 magnetization values, one for each of the samples used. For the sake of organization, only the plots and calculations for the Light Mineral Oil sample will be included in the results section. All other samples' plots are included in the **Supporting Data** section.

For each of the runs, an M_{eq} value is also found by determining the time where the signal peak reaches a maximum magnitude. This M_{eq} value is necessary to calculate the T_1 value for each of the samples. The T_1 values are detailed in **Table 1**.

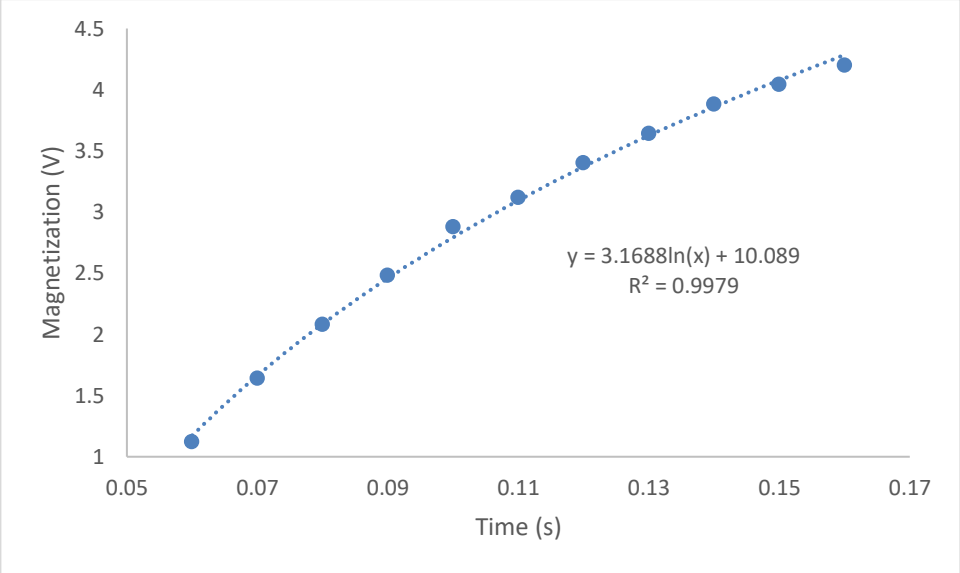


Figure 1 – T_1 data for Light Mineral Oil. The plot depicts the T_1 signal peak intensity at different times.

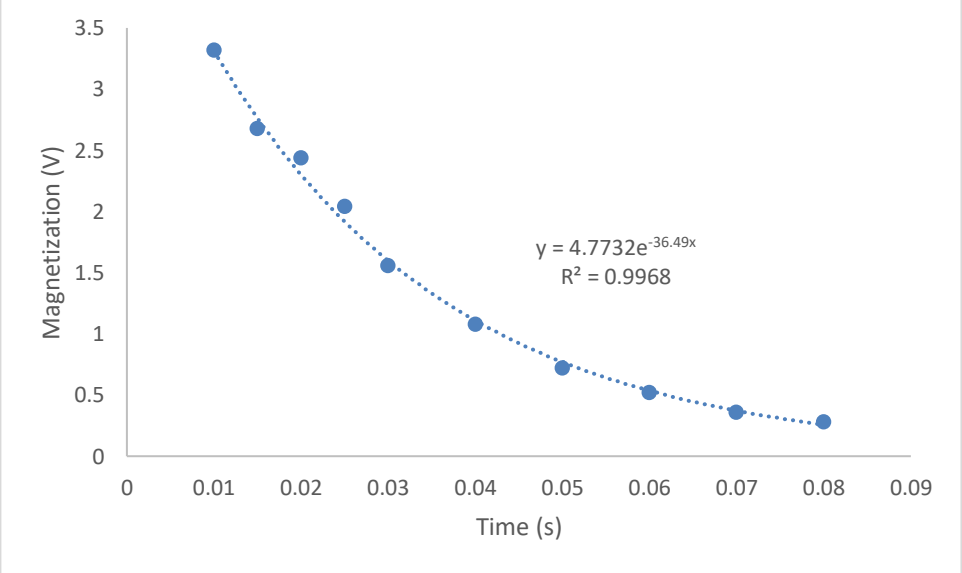


Figure 2 – T_2 data for Light Mineral Oil. The plot depicts the T_2 signal peak intensity at different times.

Table 1 – M_{eq} Values for Each Sample	
Sample	T_1 M_{eq} (V)
Light Mineral Oil	6.12

Heavy Mineral Oil	5.96
Water	1.42
Water w/ $FeCl_3$	9.30

Ideally, each of the plots should follow a trend corresponding to different equations for the T_1 and T_2 signal-time plots. The T_1 plots should mimic the equation $M(\tau) = M_{eq}\left(1 - 2e^{\frac{-\tau}{T_1}}\right)$ and the T_2 plots should mimic the equation $M_{x,y}(2\tau) = M_{eq}e^{\frac{-2\tau}{T_2}}$. By transforming these equations into the forms shown in **Calculations [1]** and **[2]**, the plots will be converted into a linear form, with the slope of both plots being equivalent to $\frac{-1}{T_x}$. As with the experimental plots, only the data for the Light Mineral Oil readings will be included here. All other samples' data will be shown in the **Supporting Data** section.

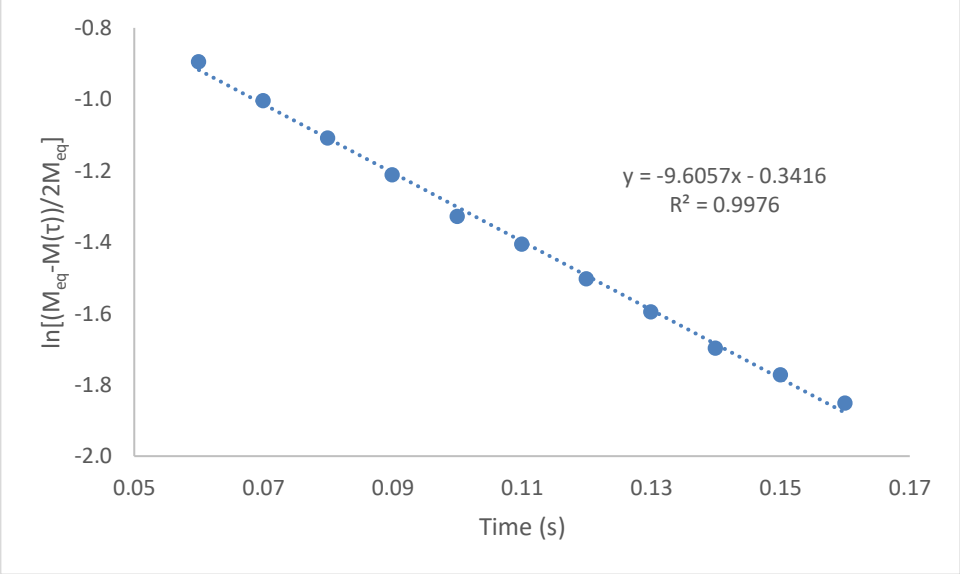


Figure 3 – Linear fit of **Figure 1** data. The slope of the trendline formed from this data is equivalent to $-1/T_1$.

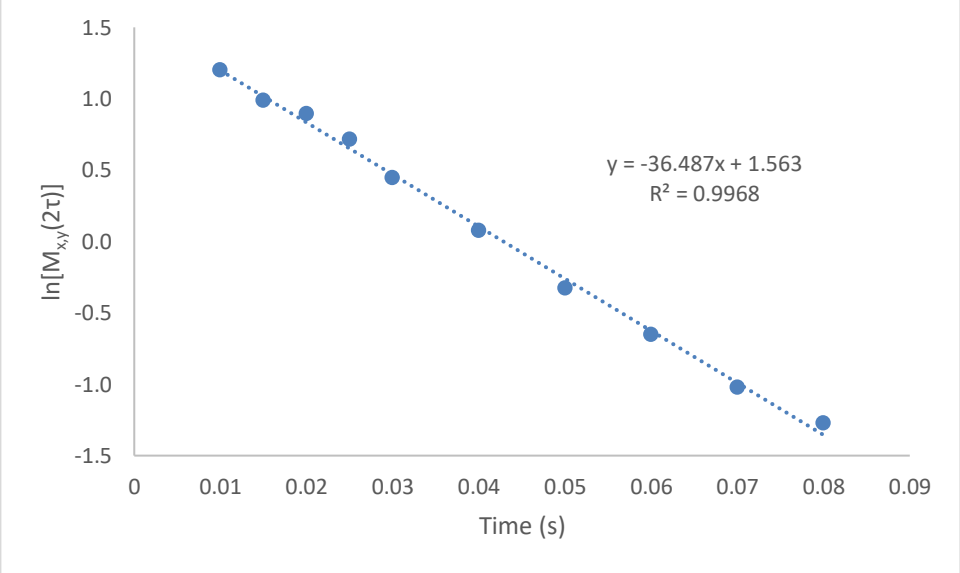


Figure 4 – Linear fit of **Figure 2** data. The slope of the trendline formed from this data is equivalent to $-1/T_2$.

The values for the slope and the uncertainty of the slope are found by using the LINEST function with the data plots. The table below details the slope and their uncertainties for all of the samples.

Table 2 – Slope Values for Linear T_1 and T_2 Data Plots		
Sample	T_1 Plot Slope and Uncertainty (s^{-1})	T_2 Plot Slope and Uncertainty (s^{-1})
Light Mineral Oil	-9.61 ± 0.2	-36.5 ± 0.7
Heavy Mineral Oil	-13.5 ± 0.6	-50.3 ± 1
Water	-0.725 ± 0.01	-12.3 ± 0.4
Water w/$FeCl_3$	-0.109 ± 0.00005	-42.2 ± 0.9

Considering that the slopes for each of these plots equate to either $-1/T_1$ or $-1/T_2$ depending on the plot, **Calculations [3]** and **{3}** can be used to determine the T_1 and T_2 values for each sample, as well as these values' uncertainties. The results from these calculations are shown below.

Table 3 – T_1 and T_2 values for each sample		
Sample	T_1 (s) [3] {3}	T_2 (s) [3] {3}
Light Mineral Oil	0.104 ± 0.002	0.0274 ± 0.0006
Heavy Mineral Oil	0.0741 ± 0.003	0.0199 ± 0.0004
Water	1.38 ± 0.03	0.0812 ± 0.003
Water w/$FeCl_3$	9.20 ± 0.003	0.0237 ± 0.0005

Sample Calculations (15 pts)

[1]

$$\frac{-\tau}{T_1} = \ln\left[\frac{M_{eq} - M(\tau)}{2M_{eq}}\right]$$

$$\langle\frac{-\tau}{T_1}\rangle_{LMO}{}_{0.06} = \ln\left[\frac{6.12\text{ V} - 1.12\text{ V}}{2 \cdot 6.12\text{ V}}\right] = -0.895$$

[2]

$$\frac{-2\tau}{T_2} + \ln[M_{eq}] = \ln[M_{x,y}(2\tau)]$$

$$\langle\frac{-2\tau}{T_2} + \ln[M_{eq}]\rangle_{LMO}{}_{0.01} = \ln[3.32\text{ V}] = 1.20$$

[3]

$$T = \frac{-1}{m}$$

$$T_{1_{LMO}} = \frac{-1}{-9.61\text{ s}^{-1}} = 0.104\text{ s}$$

{3}

$$\delta T = \left|\frac{\delta m \cdot T}{m}\right|$$

$$\delta T_{1_{LMO}} = \left|\frac{0.158\text{ s}^{-1} \cdot 0.104\text{ s}}{-9.61\text{ s}^{-1}}\right| = 0.002\text{ s}$$

Discussion, 1 (min) – 2 (max) pages, single spaced (35 pts)

As stated in the hypothesis section, it was believed that steepness of the T_1 and T_2 value curves (**Figures 1-2, Supporting Data 1-2, 5-6, 9-10**) would correspond to the hydrogen atom densities in the sample. Likewise, it was proposed that light mineral oil would show the steepest plots, followed by heavy mineral oil, and then water, and then water with $FeCl_3$. Looking at the figures alone, there is no real way to guarantee whether or not this hypothesis was prove true, as each of these plots have different time periods that the magnetizations were measured at. In order to get a better understanding of the steepness of the curves, the plots were shifted to all start at the same arbitrary point. (0 s, 0 V) This was done simply by

subtracting every data point by the samples' respective initial value for both the x and y axis. The resulting plots elaborate the steepness of the curves in an easier to interpret way.

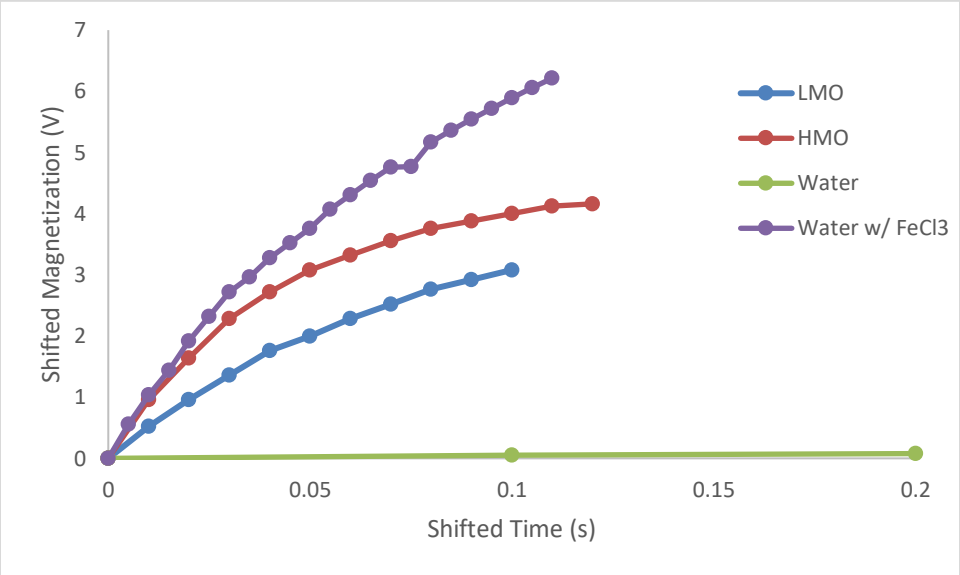


Figure 5 – Plots of T_1 values received experimentally shifted to start from point (0,0).

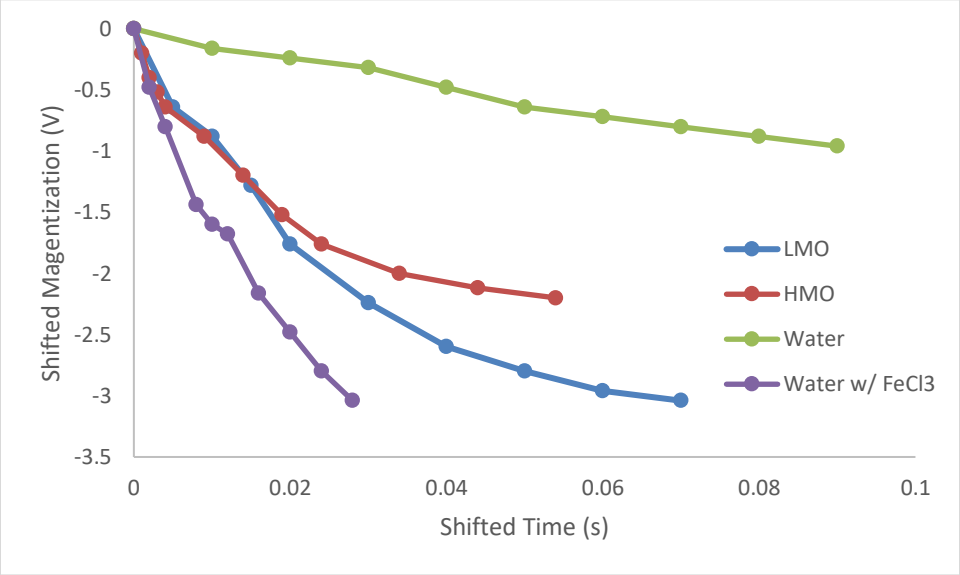


Figure 6 – Plots of T_2 values received experimentally shifted to start from point (0,0).

Both plots show that Water w/ $FeCl_3$ had the steepest change in magnetization, followed by light mineral oil, followed by heavy mineral oil, followed by water. This concludes that the hypothesis of NMR being only related to hydrogen content is false. In reality, all atoms have a magnetic moment. It can be believed that $FeCl_3$ offers a drastic shift to the overall magnetic moment of the sample.

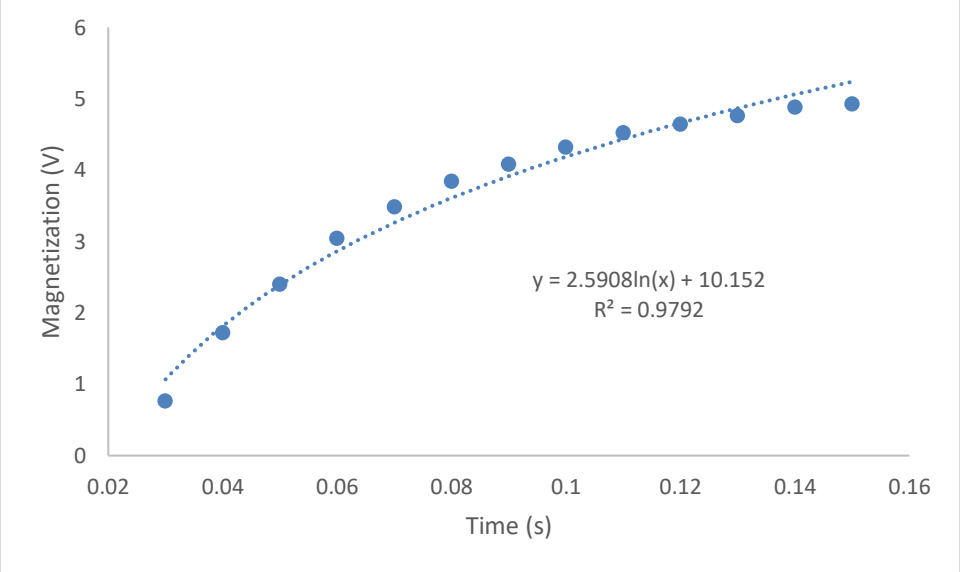
It was also believed that molecules with more hydrogens would show longer relaxation times for both T_1 and T_2. This was also proven to be false, as shown in **Table 3**. Instead it was found that water w/ $FeCl_3$ had the longest T_1 relaxation time, while water had the longest T_2 relaxation time.

The inaccuracy of these claims come from where the energy was being considered. In the hypothesis, topics and definitions were focused more on the magnetic properties of the samples. Instead, it is much easier to focus on

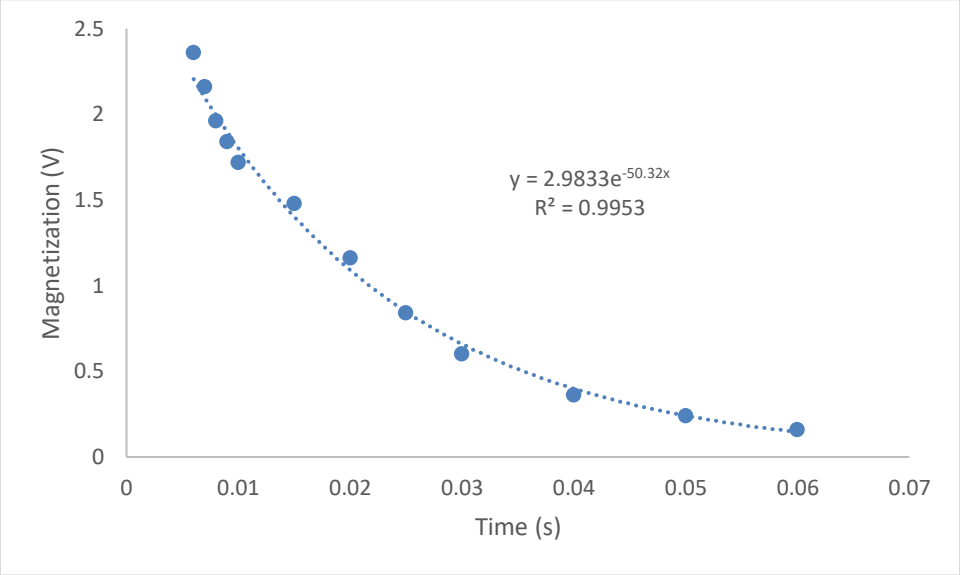
the physical motion of the atoms. Likewise, instead of focusing on the contents of hydrogen in the samples, it is better to focus on the overall size of the molecules in the sample. In the NMR system, the individual protons in the sample are forced to align to the magnetic field present in the instrument. In general, larger molecules require more energy to move the molecules around. Larger molecules imply more atoms, which imply more protons. This explains why water has the longest T_1 and T_2 relaxation times. Water molecules are very small, which mean less magnetic work is needed to get the protons to align with the magnetic field. With larger, more complex molecules like the alkanes in light mineral oil and heavy mineral oil, much more work is needed to get the protons to align with the magnetic field. Water w/ $FeCl_3$ is an exception for this case.

The reason that water w/ $FeCl_3$ is an exception in the case of the trend for both the T_1 and T_2 relaxation times is a result of ionic molecule properties. When ionic molecules are dissolved in water, the individual ions tend to separate and spread out in solution. Since the atoms have spread out, this means that the mobility of the lattice drastically increases, which results in an increase of the T_1 time. Likewise, since the ions separate, the intermolecular interactions decrease, which means T_2 decreases. This change in trend of the T_1 and T_2 values can be used to determine if there are any ions present in the solution. Basically, adding $FeCl_3$ to water increases the T_1 relaxation time drastically, while T_2 relaxation time decreases drastically, which should be accurate to if other ionic compounds were introduced to water.

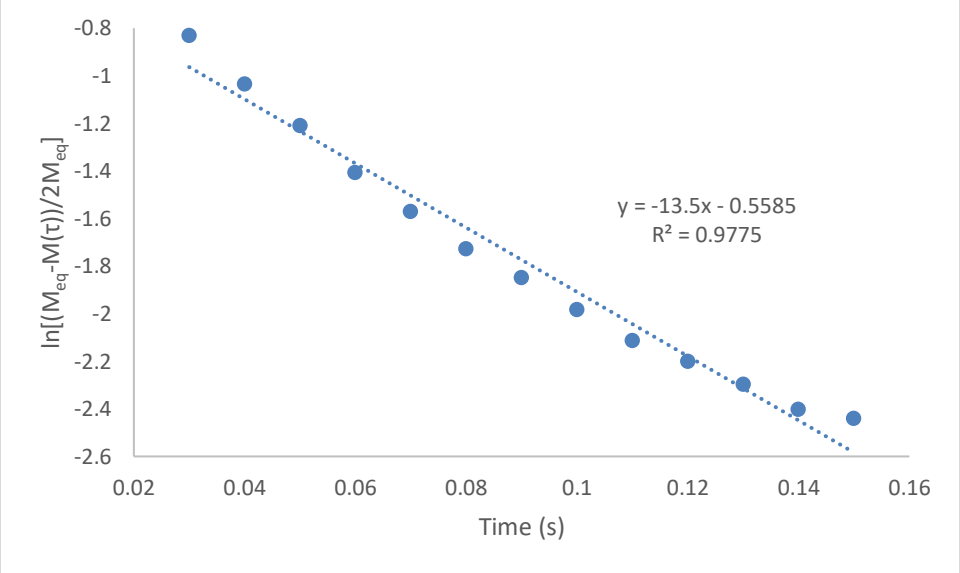
Supporting Data



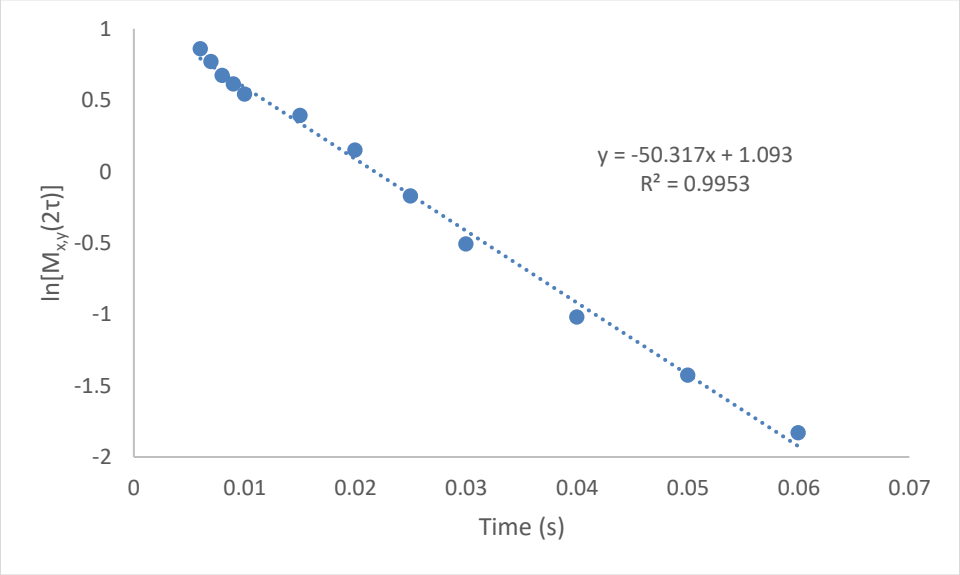
SD 1 – T_1 data for Heavy Mineral Oil. The plot depicts the T_1 signal peak intensity at different times.



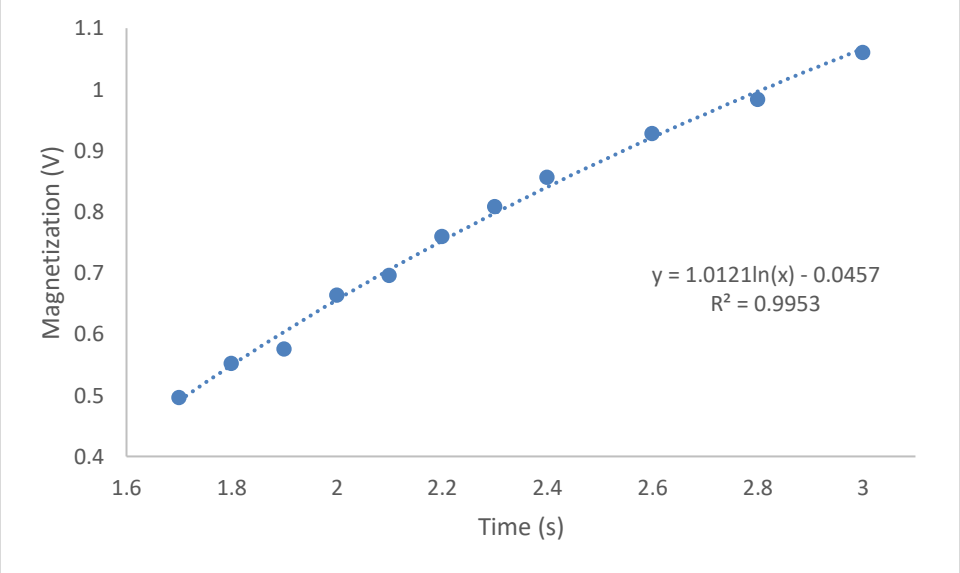
SD 2 – T_2 data for Heavy Mineral Oil. The plot depicts the T_2 signal peak intensity at different times.



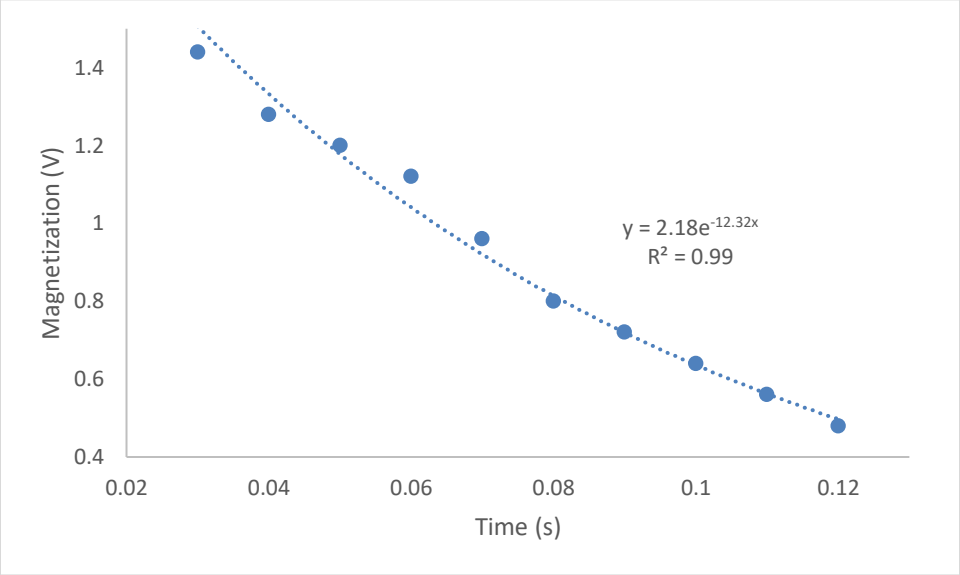
SD 3 – Linear fit of **SD 1** data. The slope of the trendline formed from this data is equivalent to $-1/T_1$.



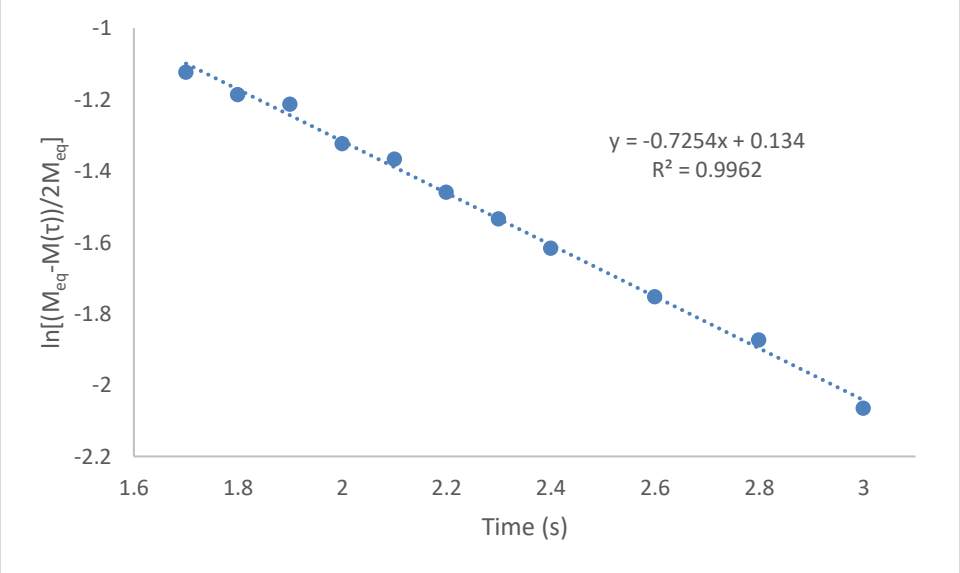
SD 4 – Linear fit of **SD 2** data. The slope of the trendline formed from this data is equivalent to $-1/T_2$.



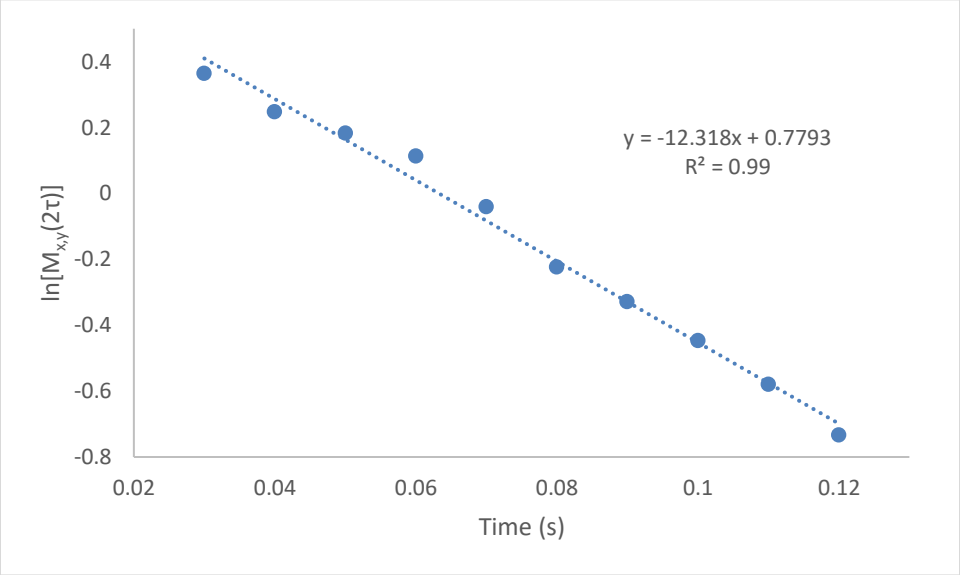
SD 5 – T_1 data for Water. The plot depicts the T_1 signal peak intensity at different times.



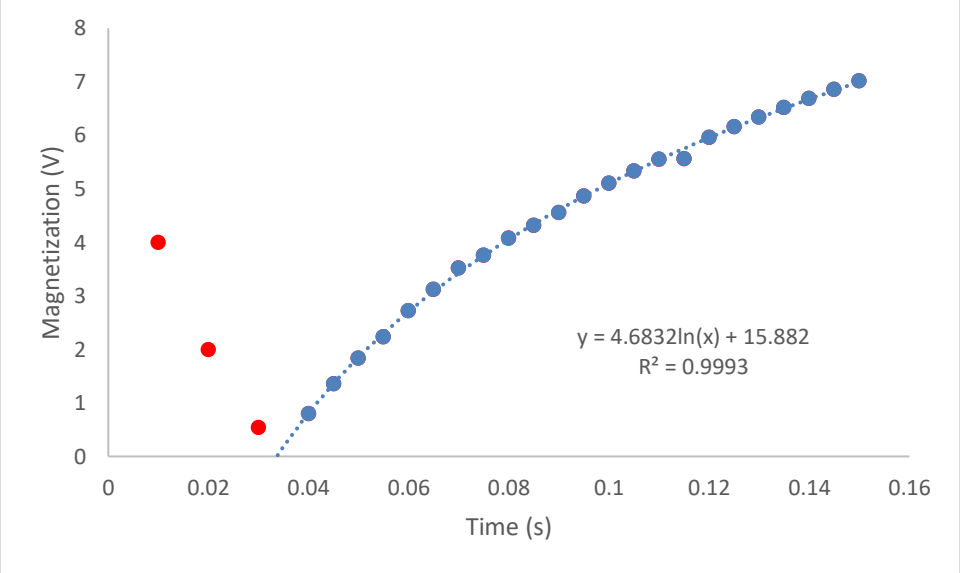
SD 6 – T_2 data for Water. The plot depicts the T_2 signal peak intensity at different times.



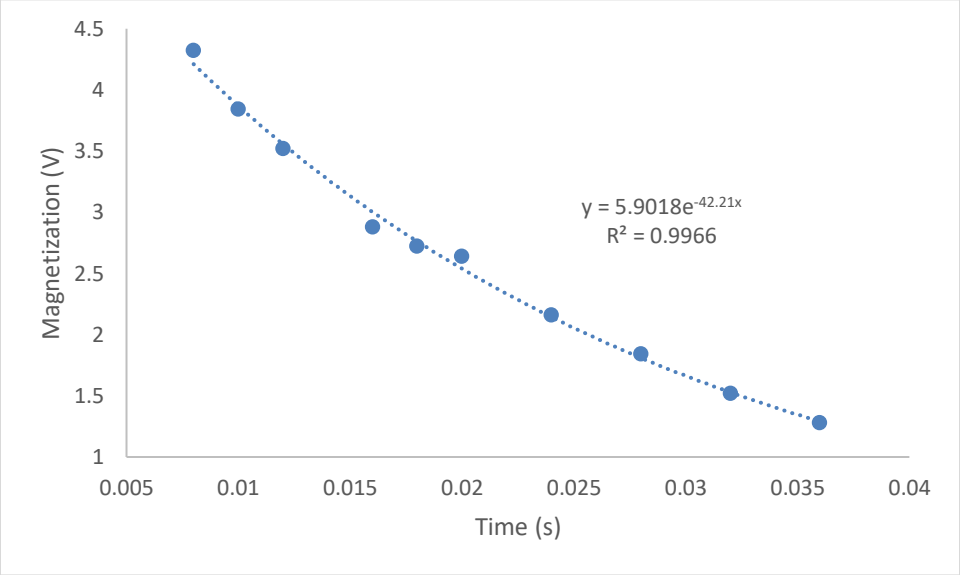
SD 7 – Linear fit of **SD 5** data. The slope of the trendline formed from this data is equivalent to $-1/T_1$.



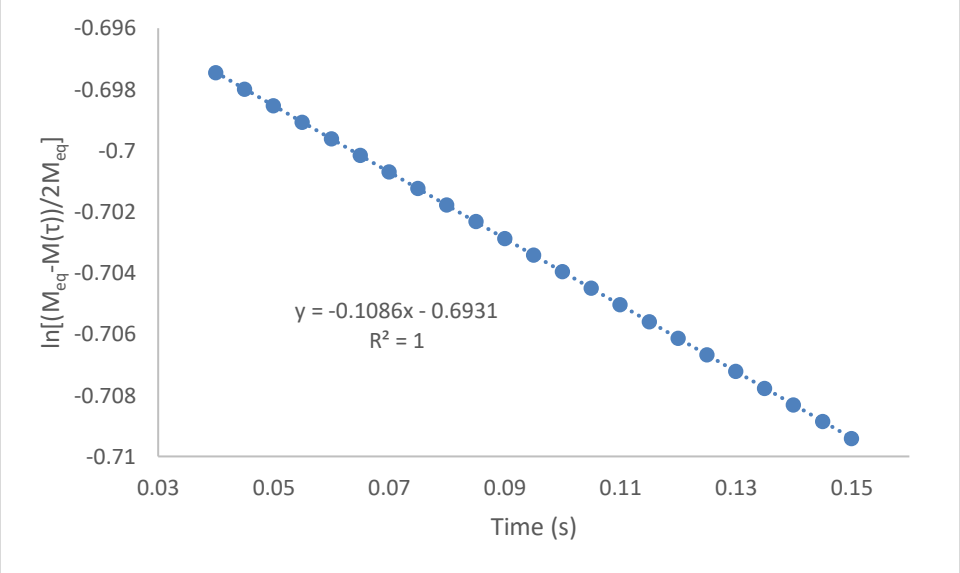
SD 8 – Linear fit of **SD 6** data. The slope of the trendline formed from this data is equivalent to $-1/T_2$.



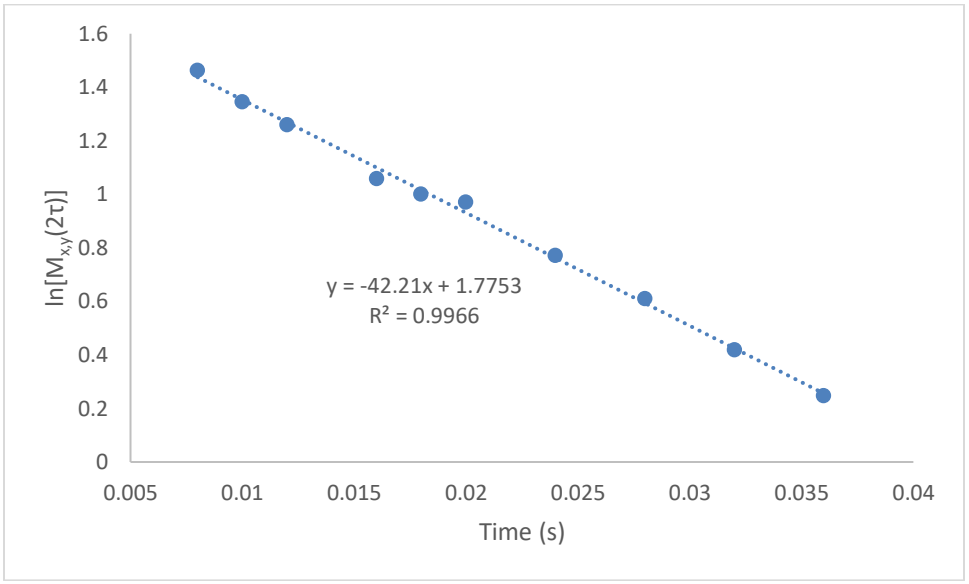
SD 9 – T_1 data for Water w/ $FeCl_3$. The plot depicts the T_1 signal peak intensity at different times. The red data points are purposefully left out of the trendline determination, and excluded from the linear fit plot.



SD 10 – T_2 data for Water w/ $FeCl_3$. The plot depicts the T_2 signal peak intensity at different times.



SD 11 – Linear fit of **SD 9** data. The slope of the trendline formed from this data is equivalent to $-1/T_1$.

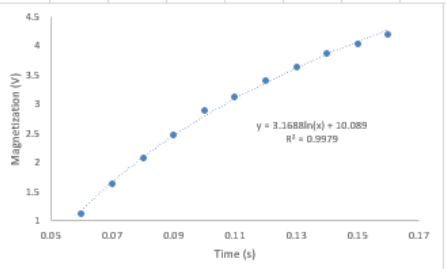


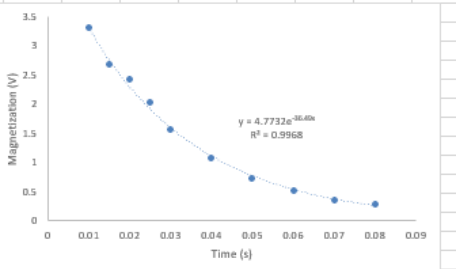
SD 12 – Linear fit of **SD 10** data. The slope of the trendline formed from this data is equivalent to $-1/T_2$.

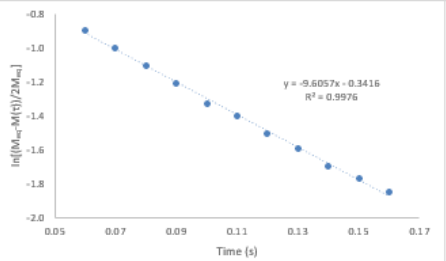
Lab Notebook

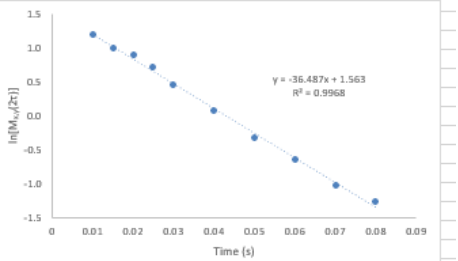
LMO

	A	B	C	D	E	F
1	Light Mineral Oil			(measuring in 10 Volt)		
2	T1			T2		
3	Tau - sec	Volts		Tau - sec	Volts	
4	0.06	1.12	-0.895	0.01	3.32	1.20
5	0.07	1.64	-1.01	0.015	2.68	0.986
6	0.08	2.08	-1.11	0.02	2.44	0.892
7	0.09	2.48	-1.21	0.025	2.04	0.713
8	0.1	2.88	-1.33	0.03	1.56	0.445
9	0.11	3.12	-1.41	0.04	1.08	0.0770
10	0.12	3.4	-1.50	0.05	0.72	-0.33
11	0.13	3.64	-1.60	0.06	0.52	-0.65
12	0.14	3.88	-1.70	0.07	0.36	-1.0
13	0.15	4.04	-1.77	0.08	0.28	-1.3
14	0.16	4.2	-1.85			
15						
16		-9.61	-0.342		-36.5	1.563
17		0.2	0.0181		0.7	0.0338
18		0.9976	0.0166		0.9968	0.0531
19	Meq	3673	9		2477.1	8
20	6.12	1.015	0.0025		6.9894	0.0226
21						
22		0.104	0.002		0.0274	0.0006
23				2.7985		
24		3.08			-3.32	
25		30.8			-43.43	
26						
27						
28						
29						
30						
31						



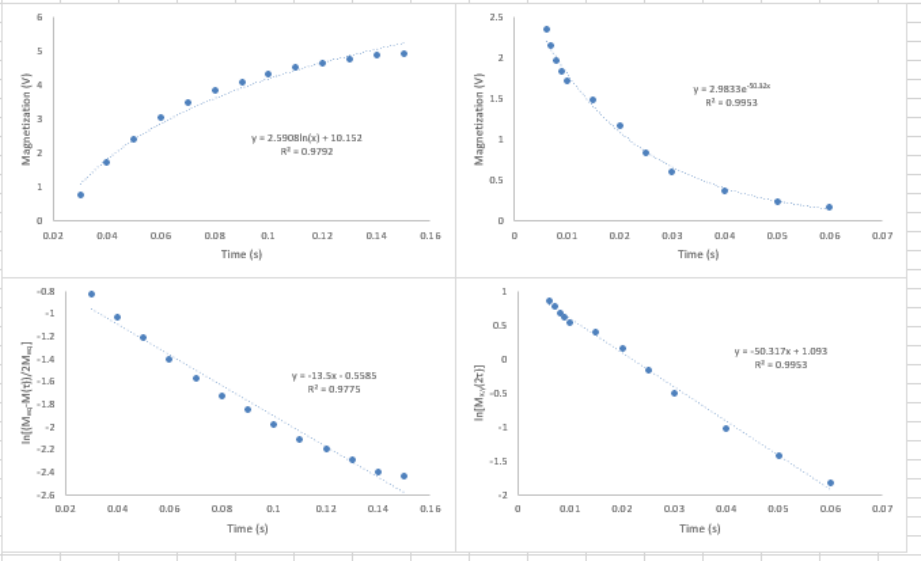






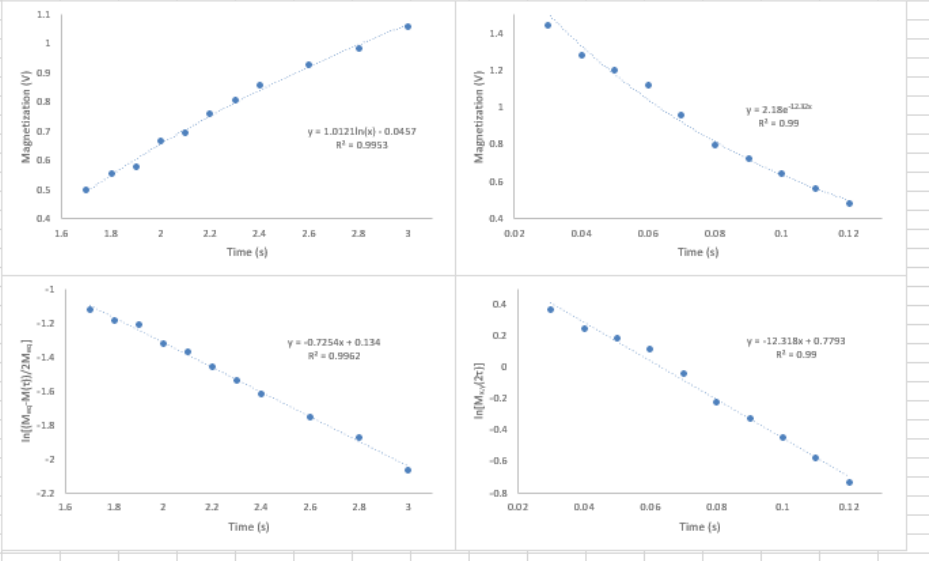
HMO

1	Heavy Mineral Oil			(measuring in 10 Volt)			
2	T1			T2			
3	Tau -sec	Volts		Tau -sec	Volts		
4	0.03	0.76	-0.83	0.006	2.36	0.8587	
5	0.04	1.72	-1.034	0.007	2.16	0.7701	
6	0.05	2.4	-1.208	0.008	1.96	0.6729	
7	0.06	3.04	-1.407	0.009	1.84	0.6098	
8	0.07	3.48	-1.57	0.01	1.72	0.5423	
9	0.08	3.84	-1.727	0.015	1.48	0.392	
10	0.09	4.08	-1.847	0.02	1.16	0.1484	
11	0.1	4.32	-1.984	0.025	0.84	-0.174	
12	0.11	4.52	-2.114	0.03	0.6	-0.511	
13	0.12	4.64	-2.201	0.04	0.36	-1.022	
14	0.13	4.76	-2.296	0.05	0.24	-1.427	
15	0.14	4.88	-2.401	0.06	0.16	-1.833	
16	0.15	4.92	-2.439				
17							
18		-13.5	-0.559		-50.3	1.093	
19	Meq	0.6	0.0602		1	0.0319	
20	5.96	0.9775	0.0833		0.9953	0.0661	
21		478.3	11		2110.2	10	
22		3.317	0.0763		9.2325	0.0438	
23							
24		0.0741	0.003		0.0199	0.0004	
25				2.7271			
26		4.16			-2.2		
27		34.667			-40.74		
28							
29							
30							
31							



Water

1	Water			(measuring in 10 Volt)			
2	T1			T2			
3	Tau -sec	Volts		Tau -sec	Volts		
4	1.7	0.496	-1.123	0.03	1.44	0.3646	
5	1.8	0.552	-1.185	0.04	1.28	0.2469	
6	1.9	0.576	-1.213	0.05	1.2	0.1823	
7	2	0.664	-1.324	0.06	1.12	0.1133	
8	2.1	0.696	-1.367	0.07	0.96	-0.041	
9	2.2	0.76	-1.459	0.08	0.8	-0.223	
10	2.3	0.808	-1.535	0.09	0.72	-0.329	
11	2.4	0.856	-1.617	0.1	0.64	-0.446	
12	2.6	0.928	-1.753	0.11	0.56	-0.58	
13	2.8	0.984	-1.874	0.12	0.48	-0.734	
14	3	1.06	-2.065				
15							
16		-0.725	0.134		-12.3	0.7793	
17		0.01	0.034		0.4	0.0352	
18		0.9962	0.0195		0.99	0.0398	
19	Meq	2384.1	9		790.44	8	
20	1.42	0.9089	0.0034		1.2519	0.0127	
21							
22		1.38	0.03		0.0812	0.003	
23				15.982			
24		0.564			-0.96		
25		0.4338			-10.67		
26							
27							
28							
29							
30							
31							



Water w/ $FeCl_3$

	A	B	C	D	E	F	G
1	Water with FeCl3				(measuring in 10 Volt)		
2	T1				T2		
3	Tau -sec	Volts			Tau -sec	Volts	
4					0.008	4.32	1.463
5	0.01	4			0.01	3.84	1.345
6	0.02	2			0.012	3.52	1.258
7	0.03	0.547			0.016	2.88	1.058
8	0.04	0.8	0.8	-0.637	0.018	2.72	1.001
9	0.045	1.36	1.36	-0.638	0.02	2.64	0.971
10	0.05	1.84	1.84	-0.639	0.024	2.16	0.77
11	0.055	2.24	2.24	-0.639	0.028	1.84	0.61
12	0.06	2.72	2.72	-0.7	0.032	1.52	0.419
13	0.065	3.12	3.12	-0.7	0.036	1.28	0.247
14	0.07	3.52	3.52	-0.701			
15	0.075	3.76	3.76	-0.701			
16	0.08	4.08	4.08	-0.702			
17	0.085	4.32	4.32	-0.702			
18	0.09	4.56	4.56	-0.703			
19	0.095	4.868	4.868	-0.703		Meq	
20	0.1	5.109	5.109	-0.704		9.30	
21	0.105	5.338	5.338	-0.705			
22	0.11	5.557	5.557	-0.705			
23	0.115	5.567	5.567	-0.706			
24	0.12	5.966	5.966	-0.706			
25	0.125	6.158	6.158	-0.707			
26	0.13	6.342	6.342	-0.707			
27	0.135	6.519	6.519	-0.708			
28	0.14	6.69	6.69	-0.708			
29	0.145	6.855	6.855	-0.709			
30	0.15	7.014	7.014	-0.709			
31							
32		-0.109	-0.693		-42.2	1.775	
33	Meq=9.3	4E-05	4E-06		0.9	0.019	
34		1	6E-06		0.997	0.025	
35		8E+06	21		2376	8	
36		3E-04	8E-10		1.437	0.005	
37							
38		3.20	0.003		0.0237	0.0005	
39				387.5			
40		3.014				3.04	
41		21.53				-108.6