W.A.R.S
WATER CONTAMINANT ANALYSIS RAMAN SPECTROMETER

CRITICAL DESIGN REVIEW
(FINAL)

Group 5
Sponsored by Ocean Insight

Our Team

George
McDonald

Photonic
Science &
Engineering

Julia
Smith-Blanchard

Photonic
Science &
Engineering

Sebastien
Jouhaud

Computer
Engineering

Gibran
Khalil

Electrical
Engineering

Juan
Restrepo Diaz

Electrical
Engineering

Water Analysis Spectrometer

- Owned by our sponsor Ocean Insight
- A spectrometer and its illumination system are important tools to help give knowledge that could not be acquired either way. It is a method of understanding molecules and how they interact with light. By analyzing the amount of light absorbed or emitted through a sample we can determine the characteristics of the sample.

Julia Smith

MOTIVATION

The overall quality of our drinking water is vital to the health and well-being of all living species on planet Earth, including humans.

Due to all the different sources of water, knowing which ones are safe to drink is essential to avoiding any kind of infections from water contaminants.

The goal behind our project is to create a water quality analyzer using Raman spectroscopy.

Julia Smith

Project Goals

The goal of this project is to build a portable, cost-effective Raman spectrometer that focuses on mainly measuring the contaminants in different water samples. Objectives are good to have to make sure that you are having standards for your project and that it is being fulfilled the prototype will meet the following goals:

- Cost
- Size
- Ease of Use

Julia Smith

Project Objectives

The **core objectives** of this project are to develop a compact spectrometer that contains simple mounted optics.

The **advanced objectives** use a combination of a well-plate reader and a detachable spectrometer to achieve a modular set-up. We will be using a 785 nm wavelength Raman laser and reduce fluoresce from signal.

George McDonald

Specifications and Requirements

Specifications	
Samples to measure	Potassium Perchlorate, Ammonium Nitrate, Sodium Sulfate
Spectral range	532 nm to 618 nm
Hardware Control	GUI fully operates well-plate motor and laser
Integration time	$\leq$ 10 seconds
Computation of Raman Spectra	Software performs image processing of Fizeau fringes
Wavelength	785 nm
Sample size	40 ml
Max laser power	40mW to 50 mW
Spectrometer dimension	3.5" x 2.5" x 1.2"
Raman spectrum resolution	20 cm^{-1}
Safety interlock engagement time	Instantaneously

Sebastien Jouhaud

Project Features

- COMPUTER APPLICATION
- CONTAMINATION DETECTION
- MODERATE SPEED
- X AND Y TABLE
- MEASURE AT LEAST 2 SAMPLES

Gibran Khalil

Work Distribution

George

Julia

- Investigate imaging techniques **(Julia – P)**
- Lens design **(George – P)**
- Contaminant research and selection **(Julia – P)**
- Spectrometer assembly and design **(George – P)**
- SHS modeling and simulation **(Julia – P)**
- Search components **(George – P)**

Sebastien

- Spectral Analysis **(P)**
- Spectrometer Research **(P)**
- C++, MATLAB, Serial Commands **(P)**
- Software integration and communication with various devices **(P)**

Gibran

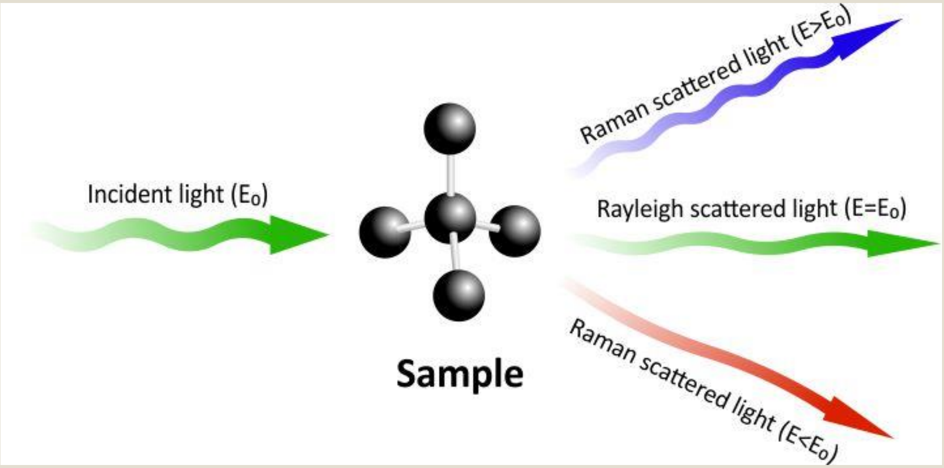
Juan

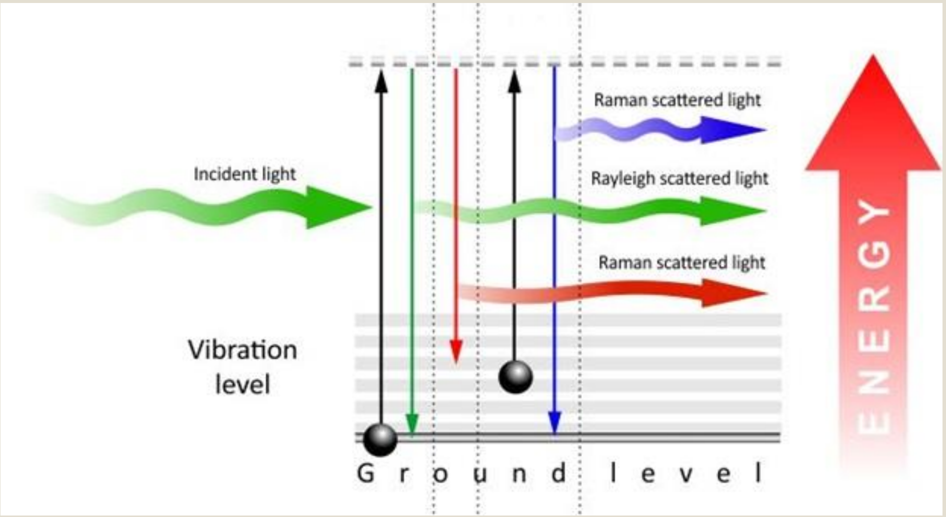
- PCB Design and Assembly **(Juan – P)**
- Power Supply Design **(Juan – P)**
- Research in humidity and thermal impact **(Juan – P)**
- System integration **(Gibran – P)**
- Precision motor design and selection **(Gibran – P)**
- Safety Design **(Gibran – P)**

Gibran Khalil

Photonics and Optics

Review on Raman Spectroscopy





Light Interaction

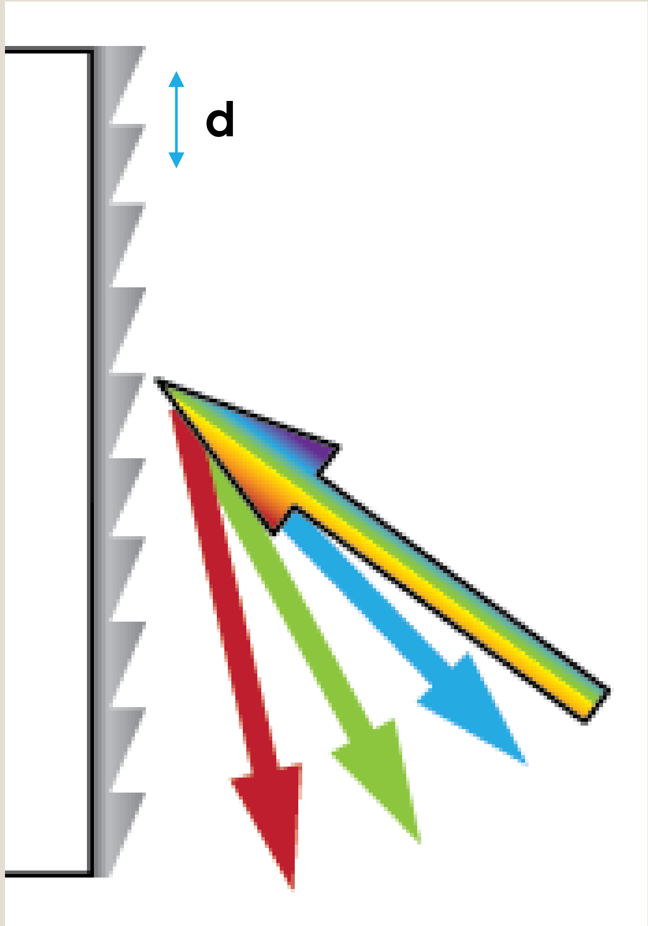
- Laser light interacts with sample
- Laser light causes molecules to vibrate in *unique* ways.
- Small fraction of light is Raman scattered.

Sample Identification

- Scattered light contains information about molecular vibrations.
- For some scattered light, there is a wavelength shift.
- Analyze intensity and wavelength to identify the material.

George McDonald

SHS Design Equations



Grating Equation: $k[\sin(\theta_L) + \sin(\theta_L - \gamma)] = \frac{m}{d}$

Littrow Angle: $\theta_L = \sin^{-1}\left(\frac{n\lambda}{2d}\right)$

Fringe Equation: $\nu_F = 4(k - k_L)\tan(\theta_L)$

Resolving Power: $R = (2)(groove\ density)(grating\ width)$

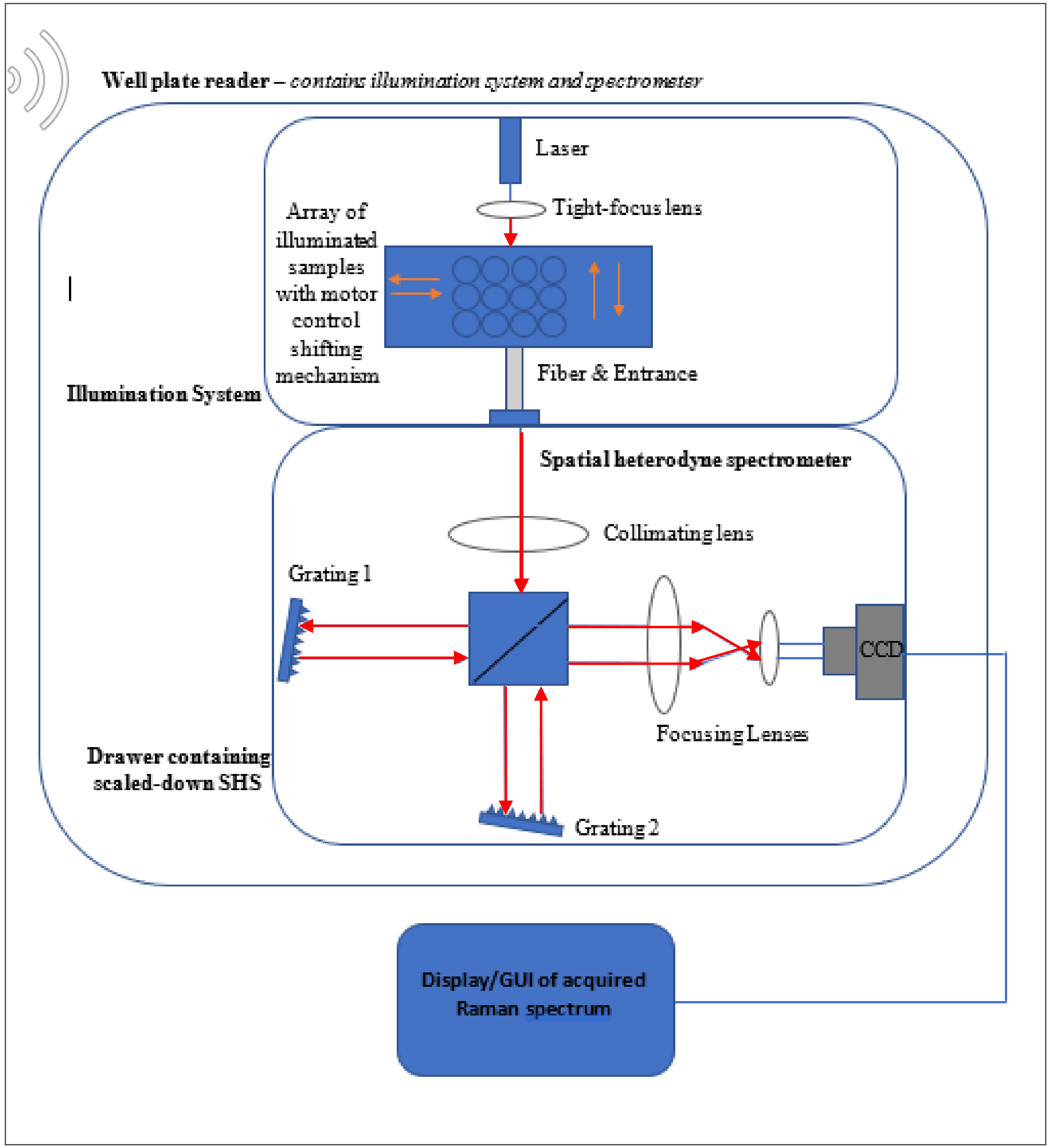
Spectral Range: $SR = \frac{(number\ of\ pixels\ along\ detector)(\lambda)}{2R}$

Resolution (nm): $FWHM = \Delta\lambda = \frac{\lambda}{R}$

Resolution (cm^{-1}): $\Delta\omega = (10^7)\frac{\Delta\lambda}{(\lambda_{exc})(\lambda)}$

Raman Shift (nm) = $\lambda = \left(\frac{1}{\lambda_{exc}[nm]} - \frac{1}{\frac{Raman\ shift\ [cm^{-1}]}{10^7}}\right)^{-1}$

George McDonald

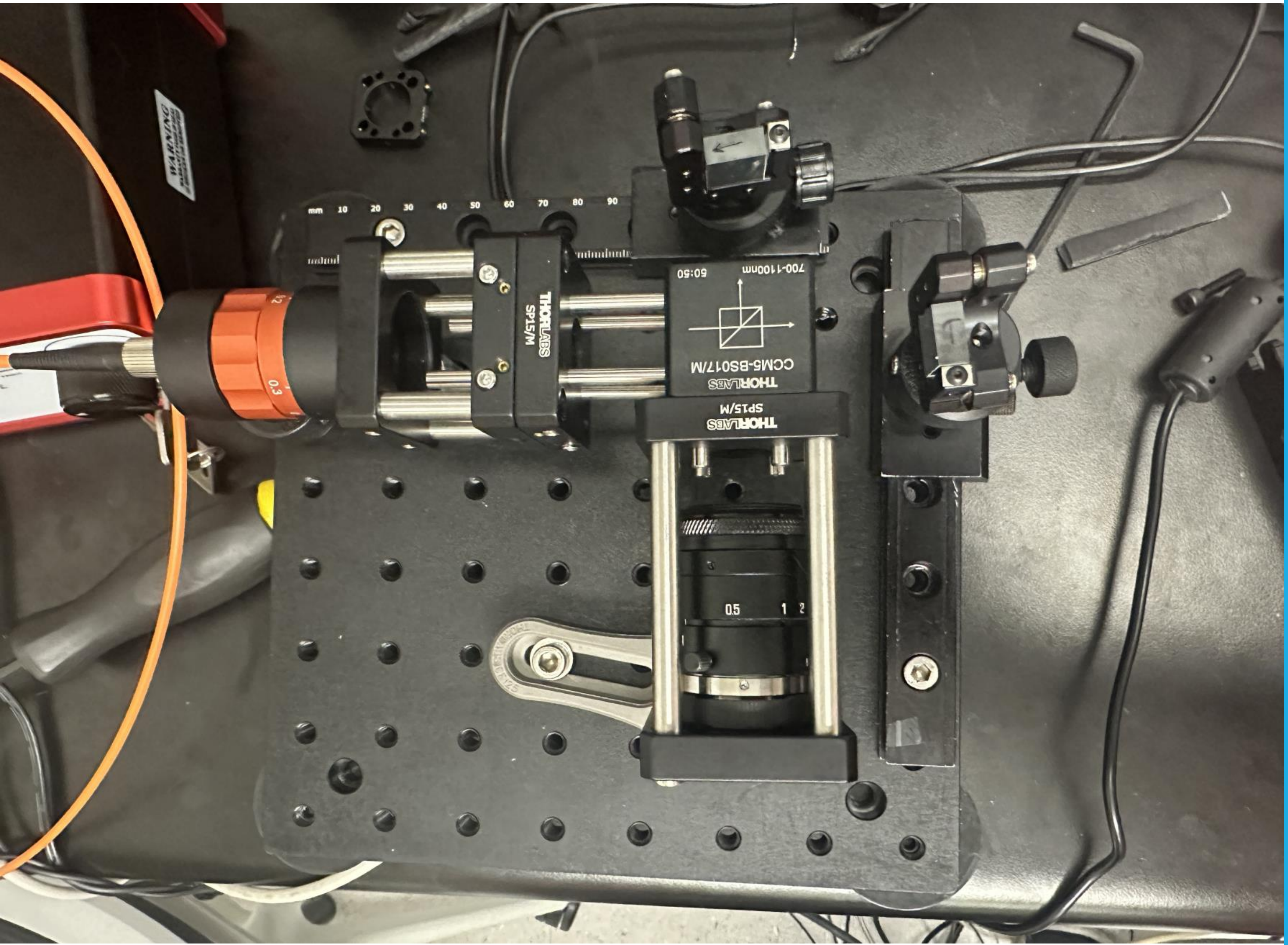


Optical Block Diagram

- **Illumination System**
  - Laser light guided to sample through emission fiber.
  - Sample is struck by laser light.
  - Collection fiber accepts scattered light.
- **SHS**
  - Accepts input light.
  - Composed of laser light, scattered light, Raman signal.
  - Scattered light splits, diffracts, and recombines.
  - Fringe image lands on detector to be processed.

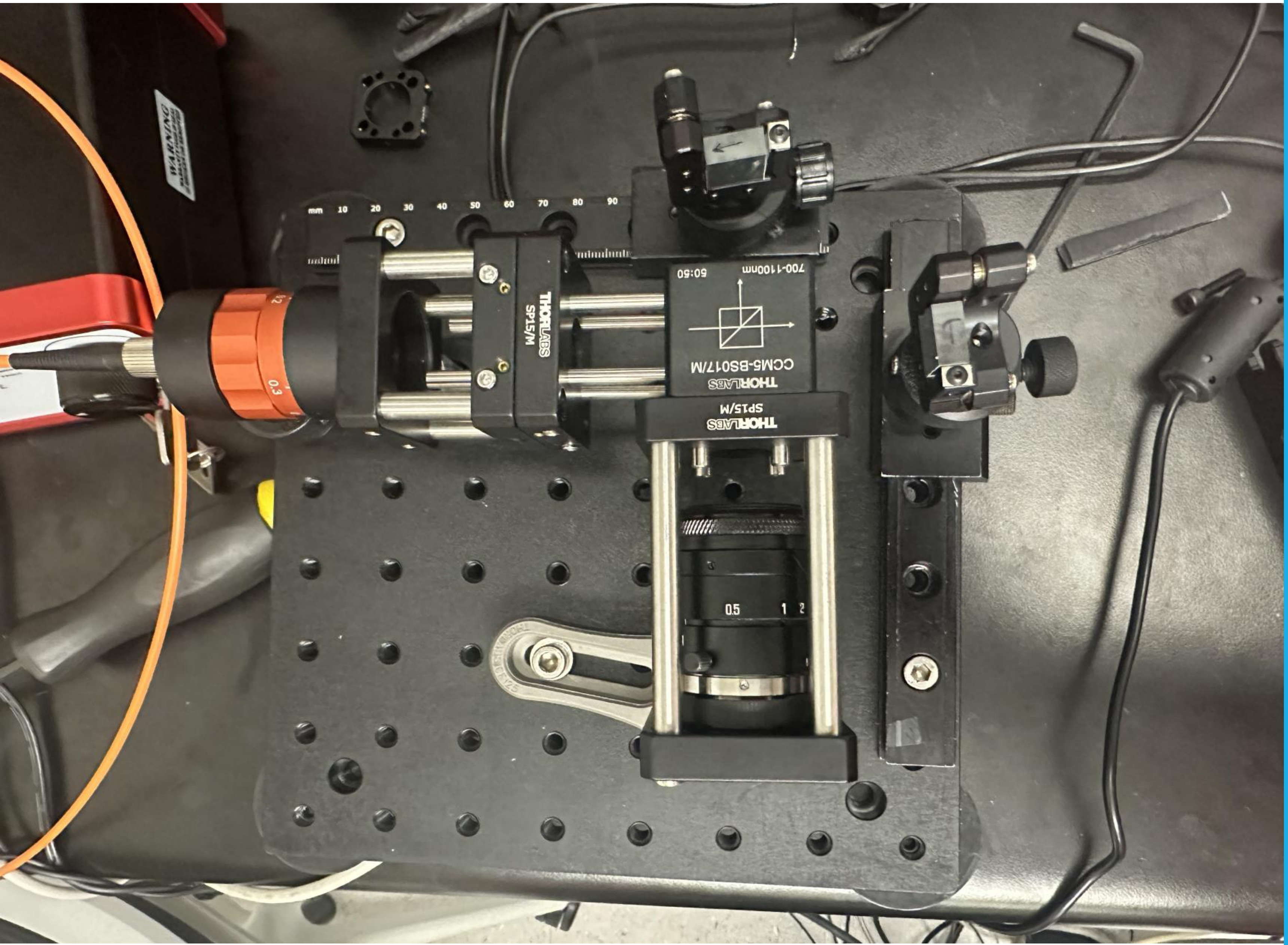
Red arrows = light propagation

Julia Smith



OPTICAL SYSTEM

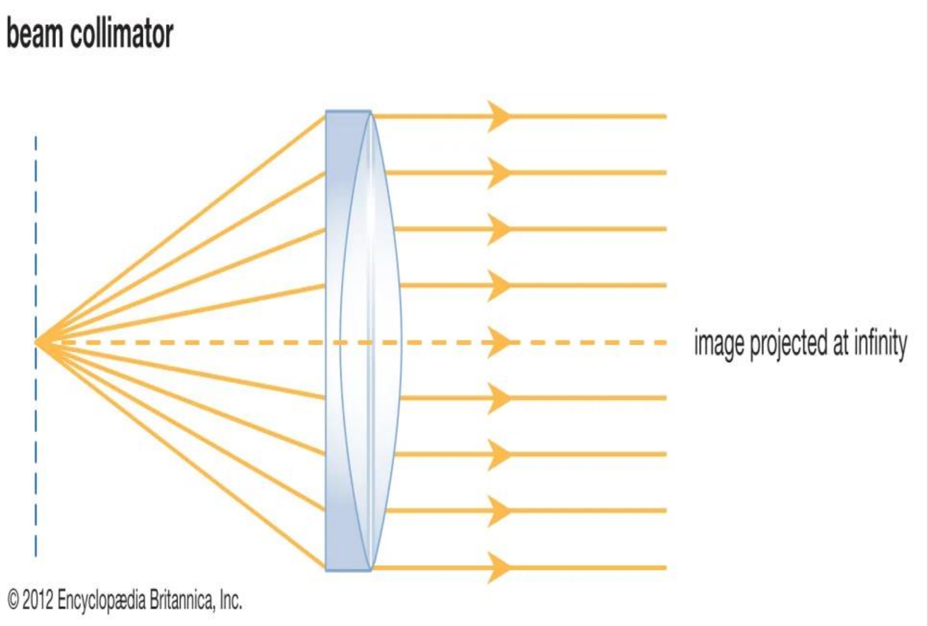
Julia Smith



OPTICAL SYSTEM

Julia Smith

Optical Component- Collimator Design



C20SMA-B - Achromatic Fiber Collimator, f = 20 mm, 650 - 1050 nm

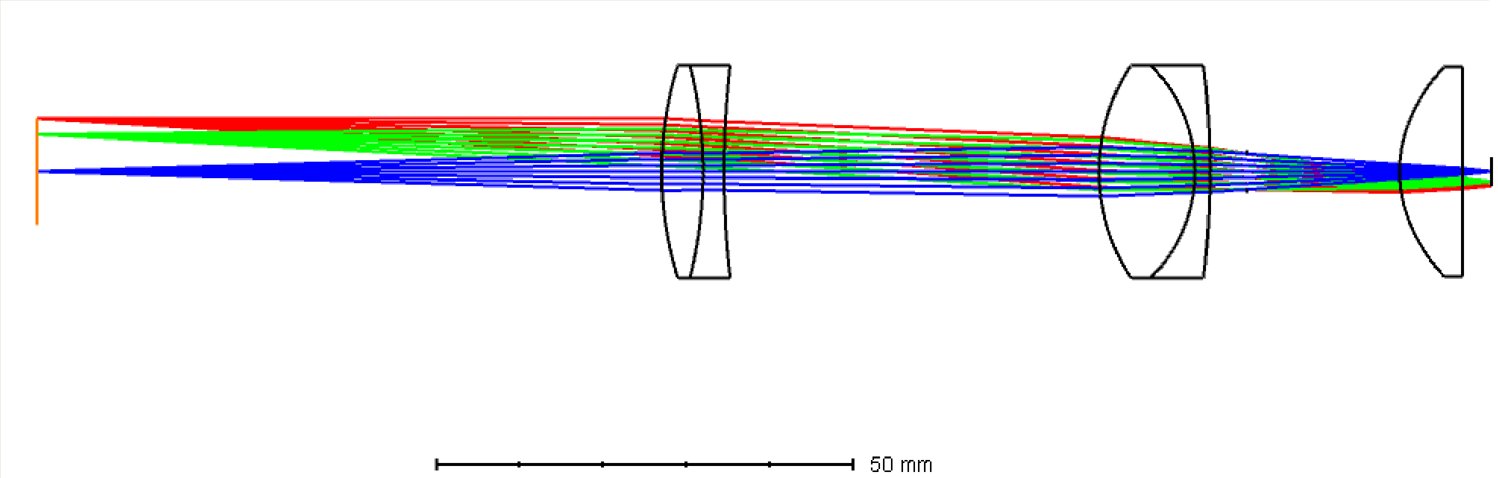
- A collimator lens is important design of the spectrometer because it changes the diverging point source to a parallel beam.

Julia Smith

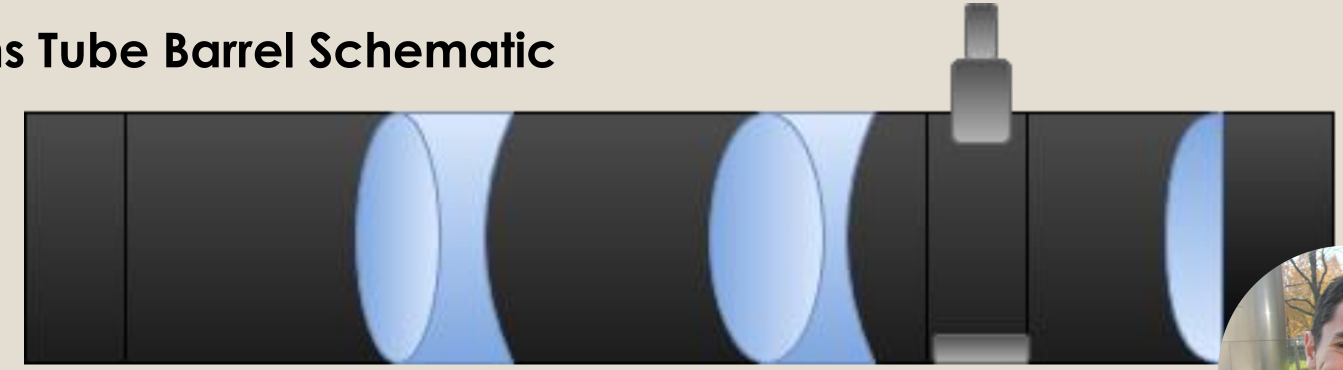
Optical Component- Imaging Design

Zemax Design

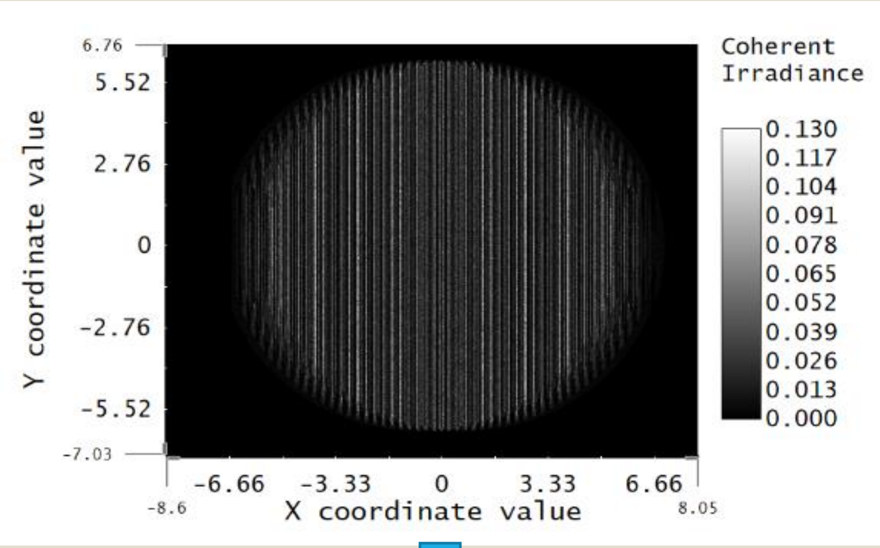
- Working Distance: ~75mm
- Image Distance: ~ 3.4mm from last surface
- Total optical track length: 99.6mm
- Effective Focal Length: 53.21mm



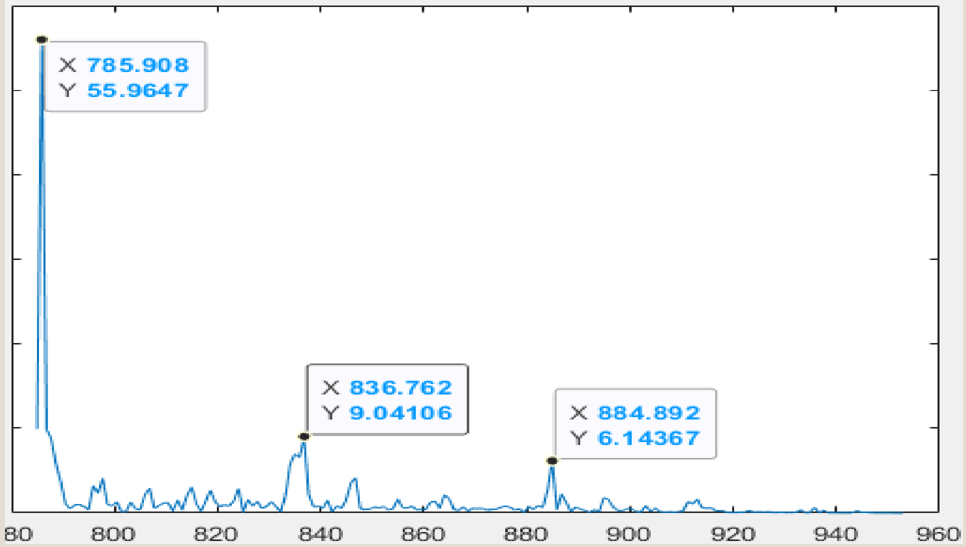
Lens Tube Barrel Schematic



George McDonald



Inverse Fourier Transform



Optical Simulation and Inverse Fourier Transform Result

- **ZEMAX**
  - Input three wavelengths into non-sequential ray trace.
    - 785 nm, 830 nm, & 885 nm
- **MATLAB**
  - Image processing
  - *Note*: Wavelength axis (x-axis) is configured to scale yet.

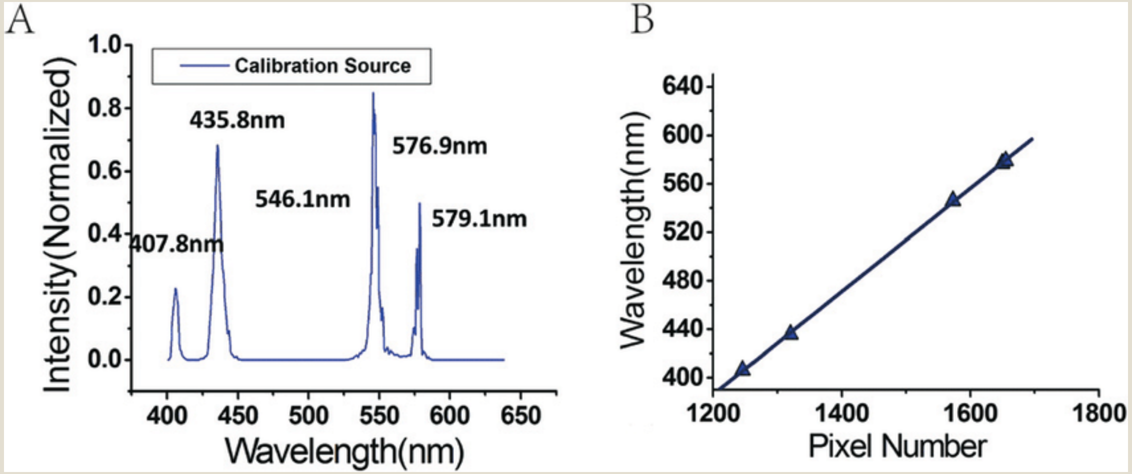
Julia Smith

Testing and Verification - Calibration

- Calibration using known light sources.
  - Light source must be within the anticipated spectral range.
  - Light source must be a line source.
- Selected light source:
  - Mercury – Contains wavelengths in the expected spectral range of spectrometer with a great peak at 546nm.

Procedure:

- Insert light source, inspect fringes, Fourier transform, plot peaks against number of pixels on detector.
- Pick three peaks (statistical minimum).
- Determine pixel position of the peak. (x-axis is pixel position, y-axis is known peak position in nm)
- Acquire linear calibration curve (y = mx + b)
- Insert pixel number into x and retrieve y value.

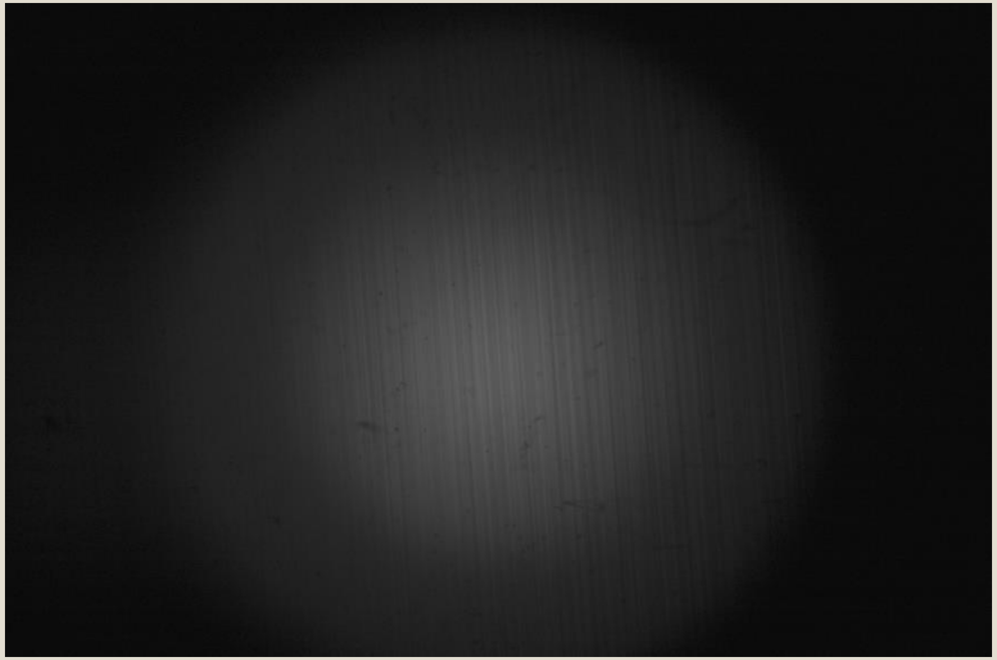


Calibration using a mercury-argon source

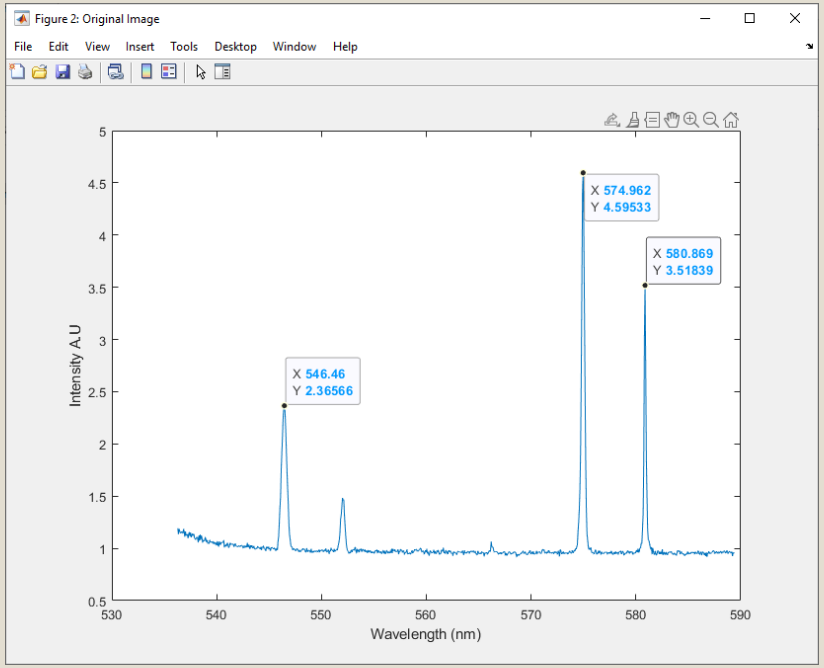
George McDonald

Testing and Verification: Resolving Power and Spectral Range

- **Mercury**
  - Resolving Power $= 2wd = 2 \times (10mm) \times 300 \frac{l}{mm} = 6000$
  - Spectral Range$= \frac{N\lambda}{2R} = \frac{(1944)(532nm)}{(2)(6000)} =$ ***86.184 nm*** -> ***2620.58*** cm^{-1}
  - Resolution $= 0.4683$nm



Fringes that result from Mercury captured by our SHS

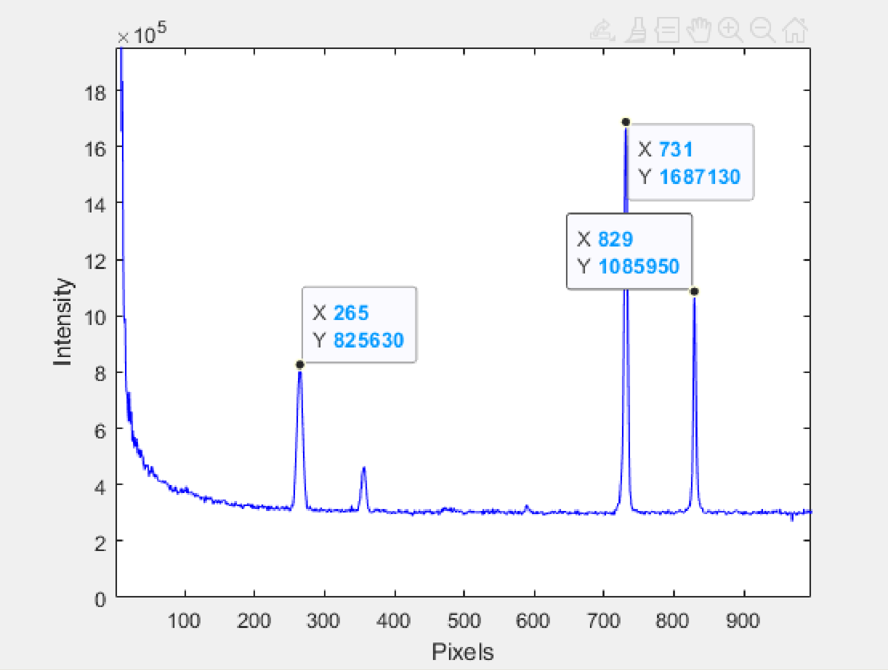


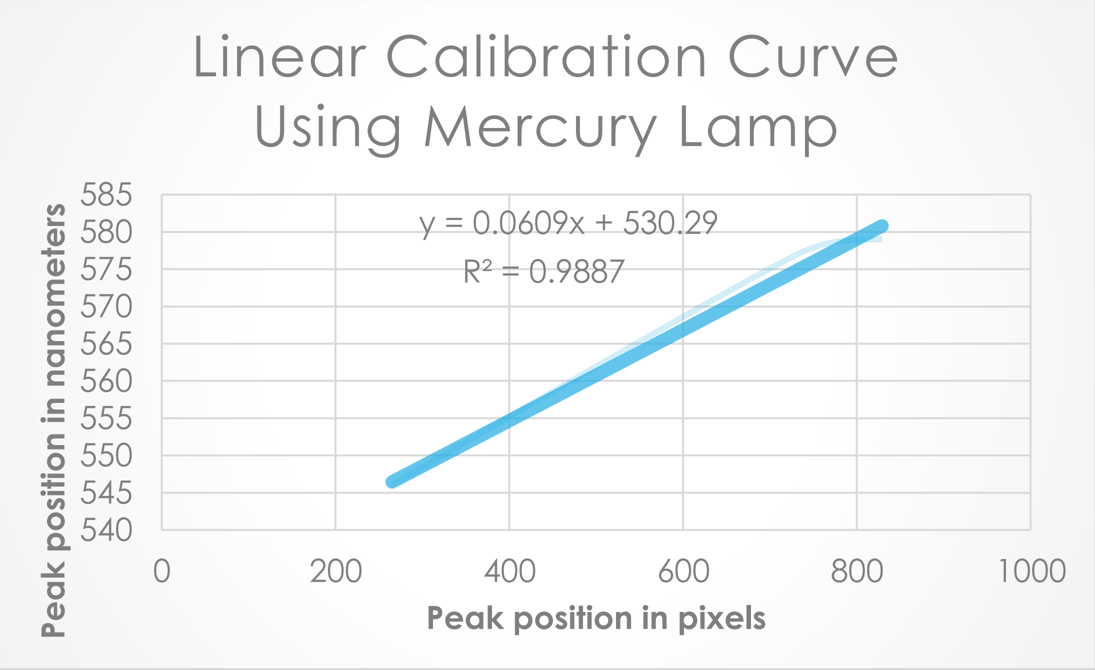
Fourier transform of fringes

George McDonald

Testing and Verification - Calibration

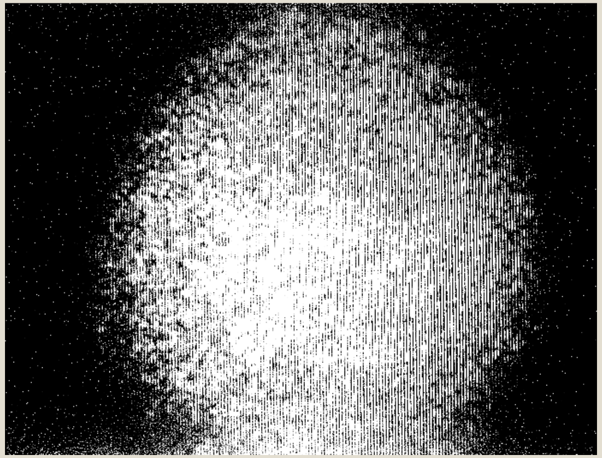
- **Mercury**
  - Known peaks: 546nm (265px), 576nm (731px), and 579nm (829px)
  - $R^2 = 0.9887, \quad y = 0.0609x + 530.29$
  - Note: Peaks that shift by $800cm^{-1}$ and lower are weak and our SHS may not be sensitive enough to pick them up. Calibration is also not perfectly set.

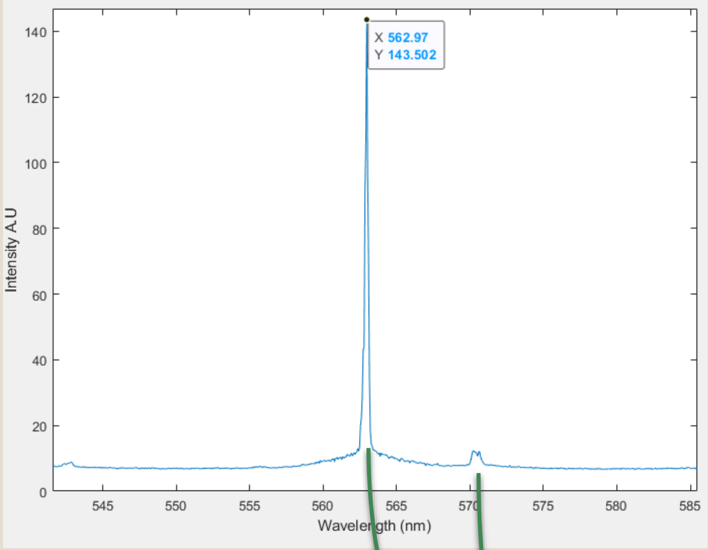




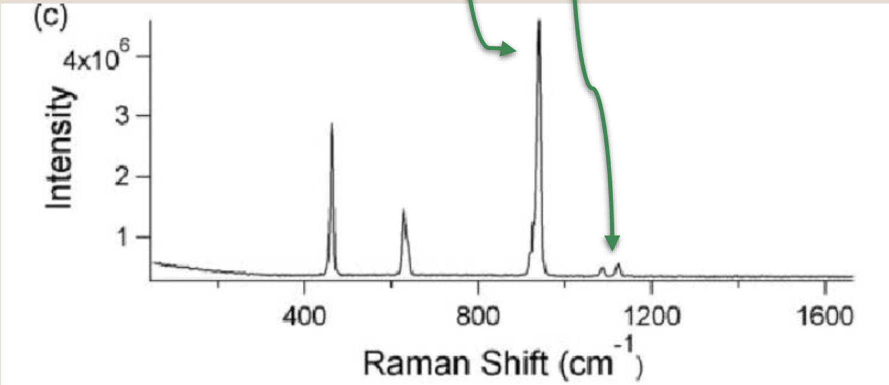
George McDonald

Measurements – Potassium Perchlorate





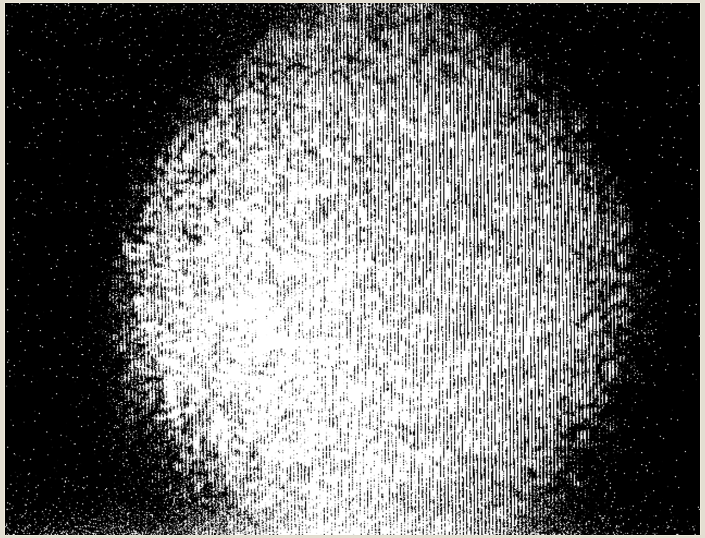
- Two significant peaks observed in the Potassium Perchlorate spectrum.
    - In upper plot: around 940 cm^{-1} peak and a peak around 1060 cm^{-1}
- Mentioned previous slide, note that peaks that shift by 800cm^{-1} and lower are weak and our SHS may not be sensitive enough to pick them up. Calibration is also not perfectly set. However, looking at the wavelength ~543nm, you can see that there is a peak with slight intensity of about 8.8 au.



Raman spectrum of KCL04: https://www.researchgate.net/figure/a-The-typical-column-summed-FT-applied-to-potassium-perchlorate-Raman-with-the_fig4_311627976

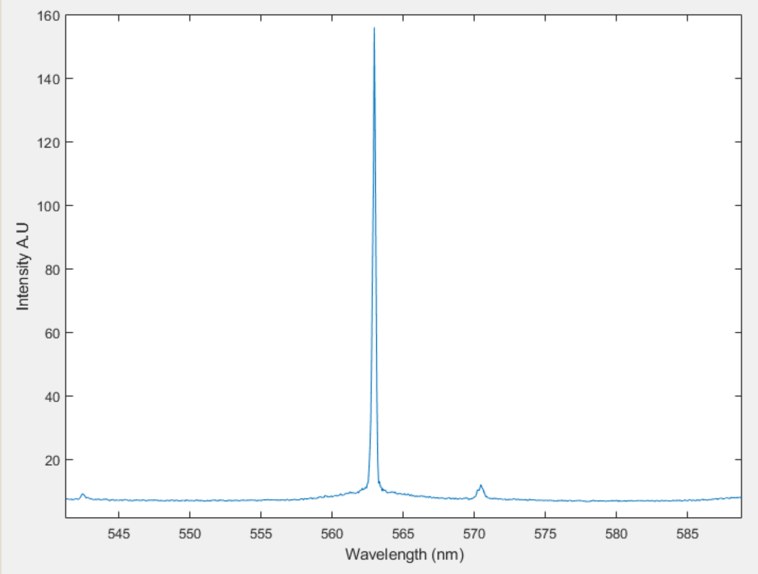
George McDonald

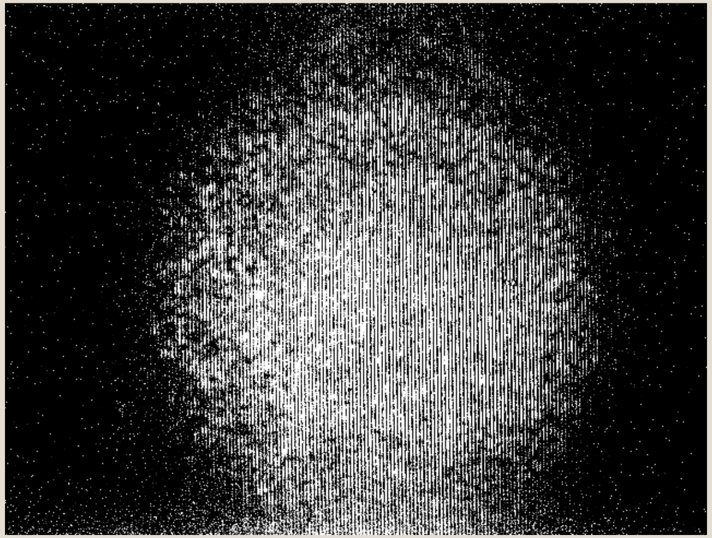
Measurements – Potassium Perchlorate



1750mg/ml

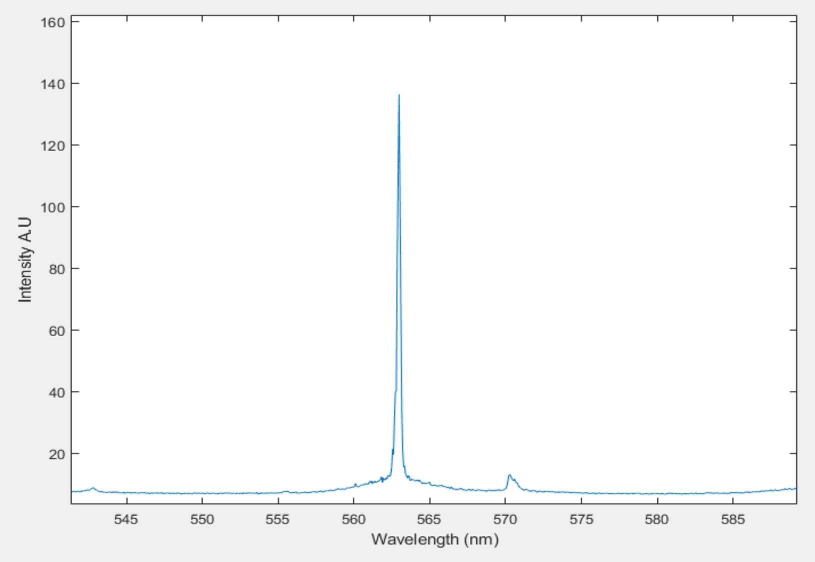
Exposure Time: 10 seconds





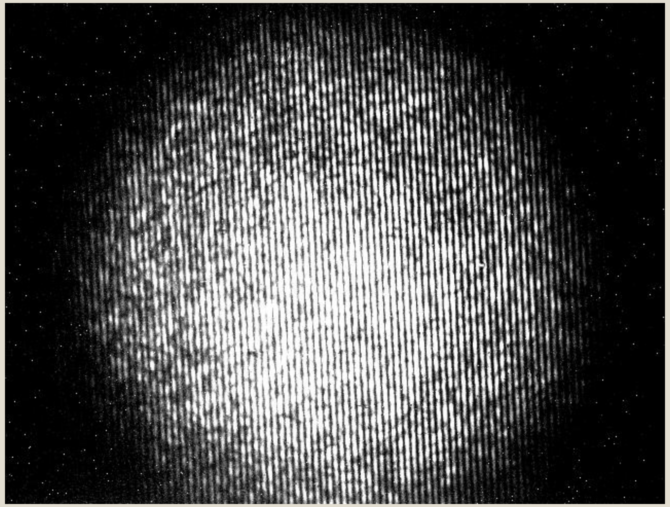
550mg/ml Concentration

Exposure Time: 10 seconds

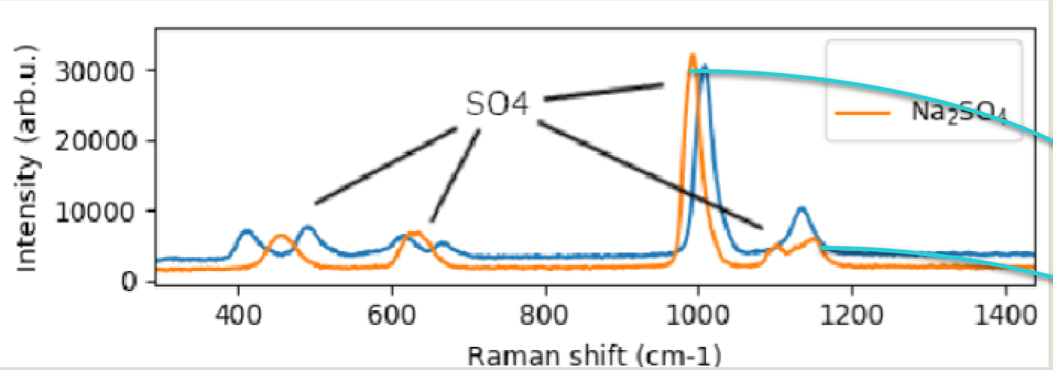


George McDonald

Measurements – Sodium Sulfate

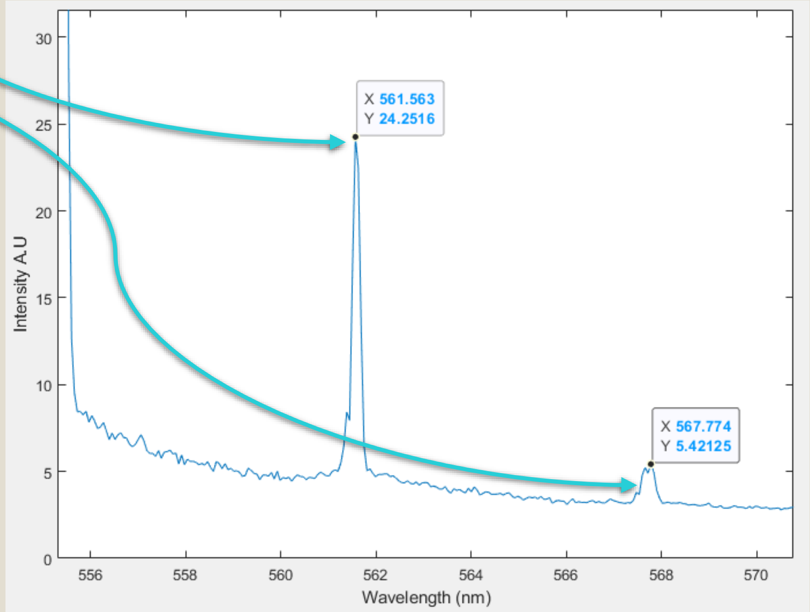


Orange line in comparison spectrum is Sodium Sulfate. Our Raman shift is only about 1000 cm^{-1} and above.



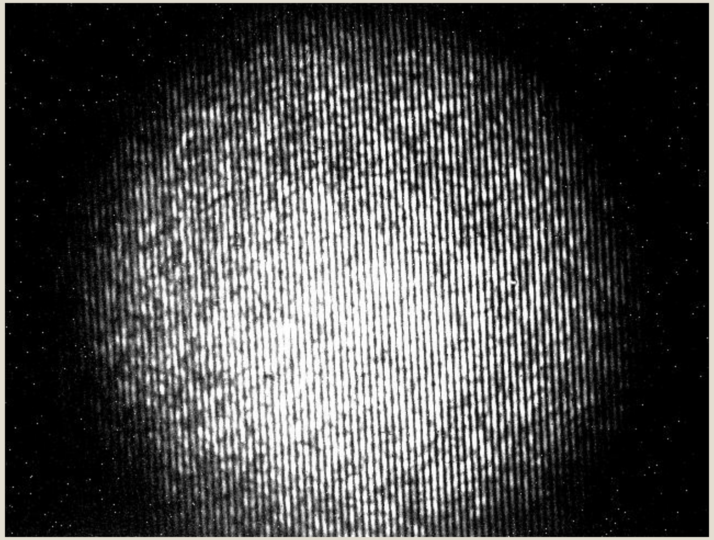
Raman spectrum of Sodium Sulfate. Image taken from *https://www.researchgate.net/figure/Example-Raman-spectra-of-CaSO-4-and-Na-2-SO-4-Both-show-typical-sulphate-Raman-modes*

- **Two significant peaks** observed in Sodium Sulfate spectrum.
  - In upper plot: around 993 cm^{-1} peak and a doublet around 1102 cm^{-1}
- 993 cm^{-1} shift from 532nm corresponds to ~561 nm. 1102 cm^{-1} and 1132 cm^{-1} corresponds approximately 565 nm and 566 nm.



Julia Smith

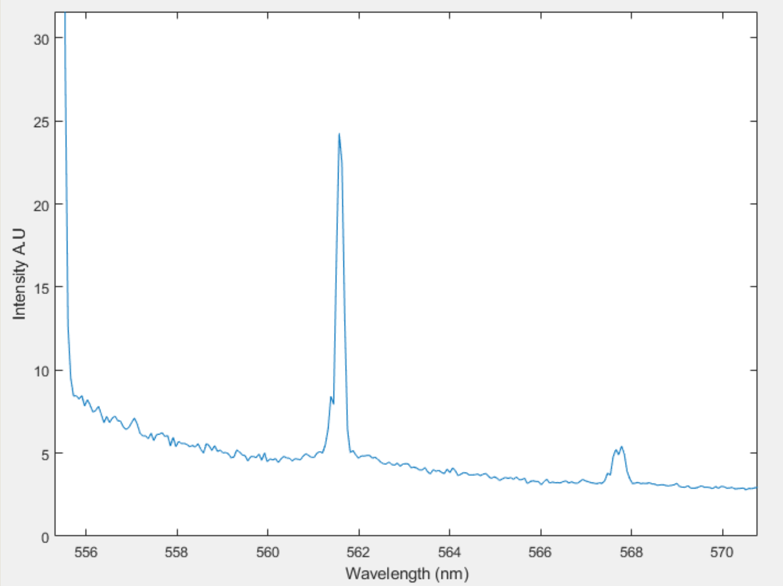
Measurements – Sodium Sulfate

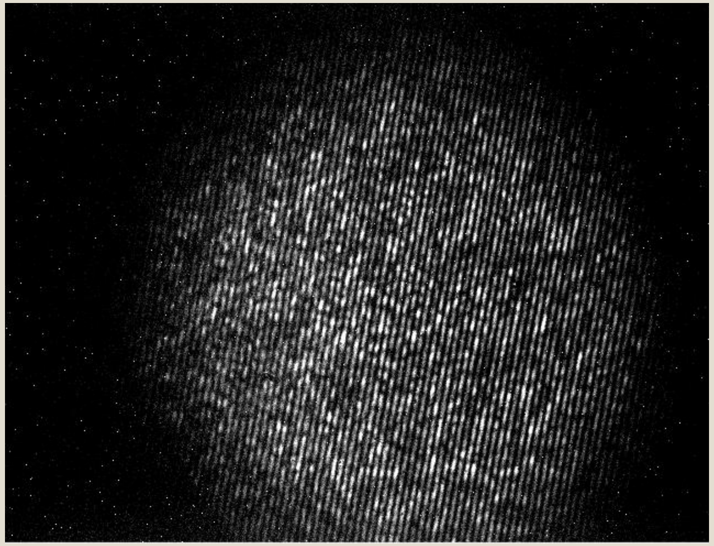


Larger concentration

1750mg/ml

Exposure Time: 10 seconds

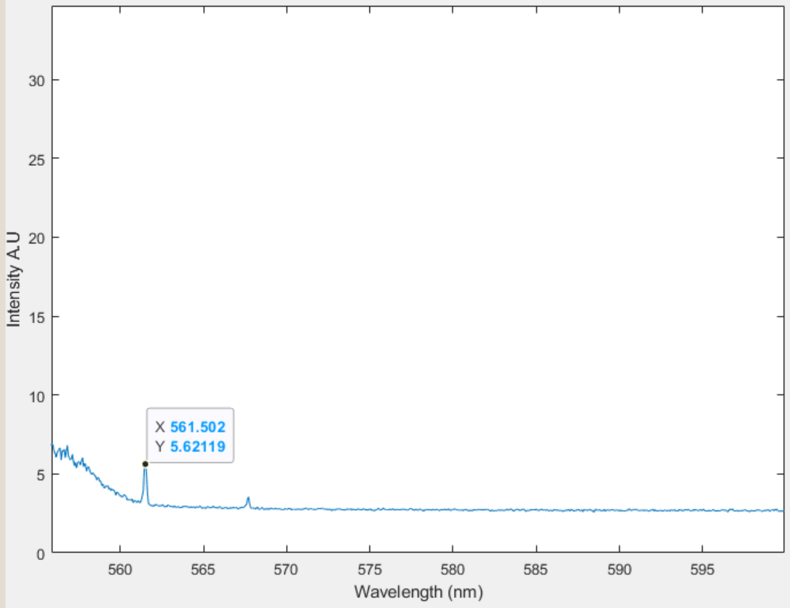




Smaller Concentration

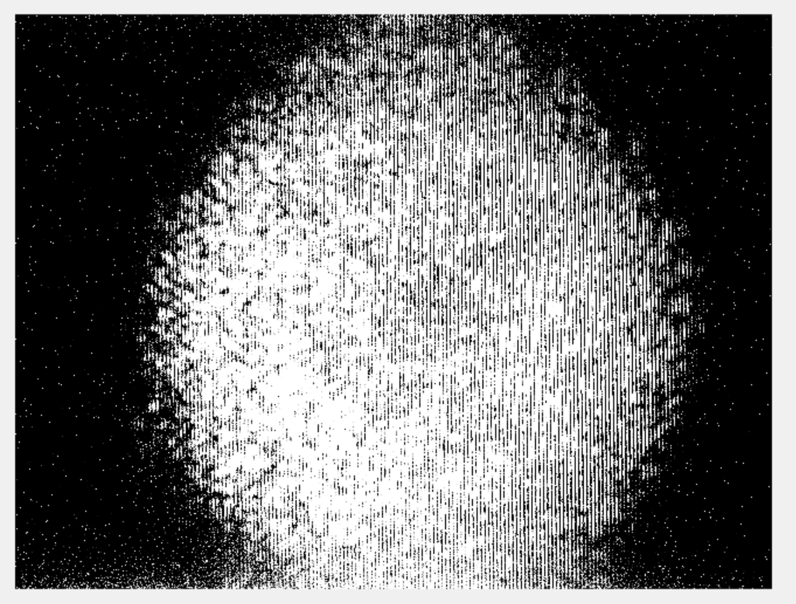
550mg/ml

Exposure Time: 10 seconds

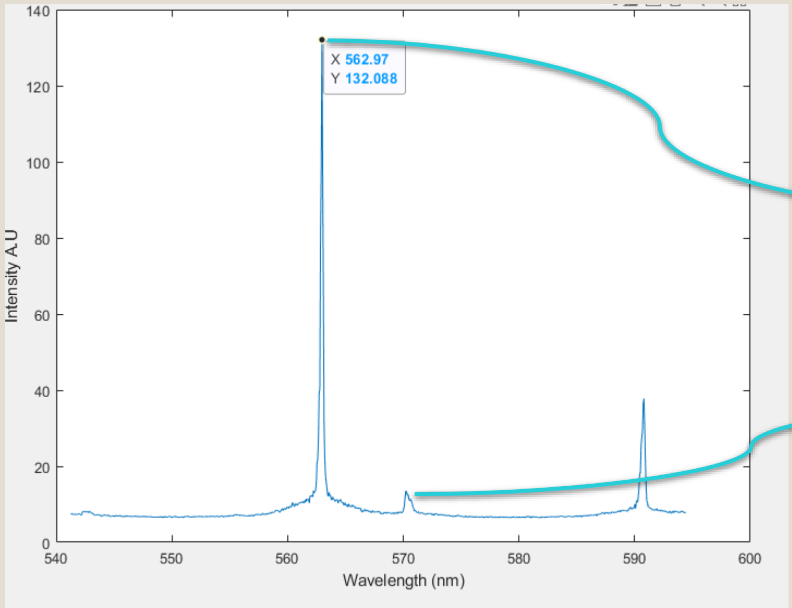


Julia Smith

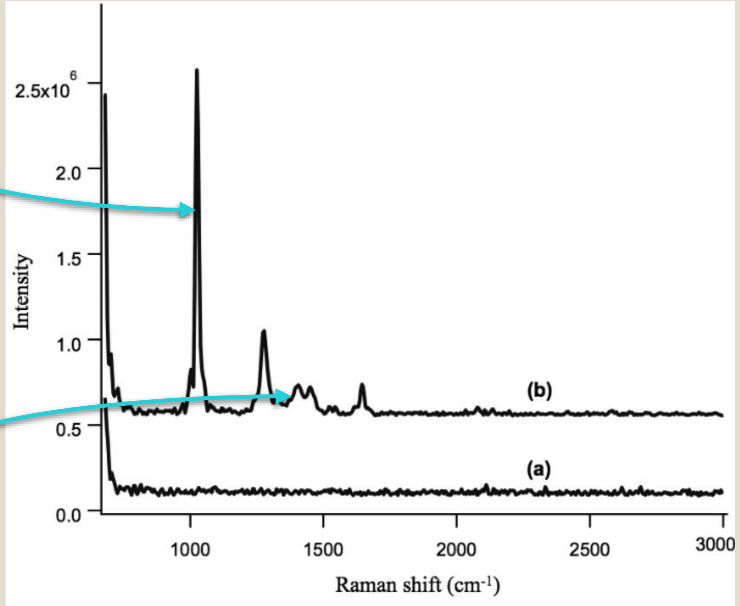
Measurements: Ammonium Nitrate



Fringes resulting from Ammonium Nitrate



Fourier transform of previous fringes



Reference spectrum: https://www.researchgate.net/figure/Spatial-heterodyne-Raman-spectra-of-ammonium-nitrate-a-Focused-25-lm-diameter-laser_fig5_274093887

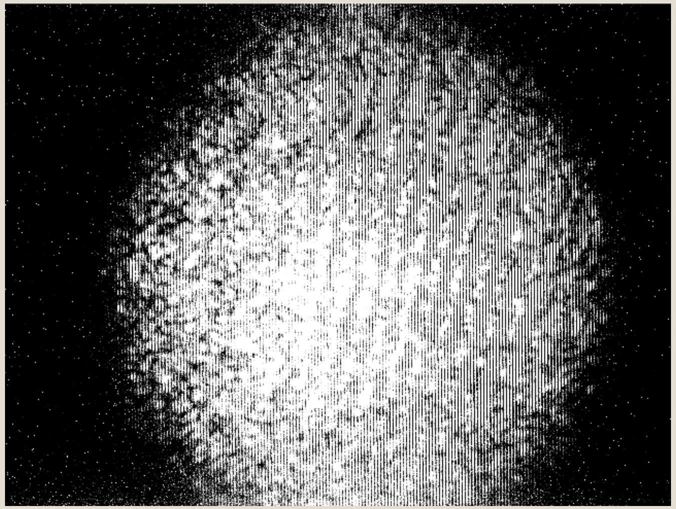
- Three significant peaks observed in Ammonium nitrate spectrum.
  - In rightmost plot: 1046cm^{-1} peak, 1250cm^{-1} peak, and a peak shy of 1450cm^{-1}

- 1046cm^{-1} shift from 532nm corresponds to ~561nm. In middle plot, largest peak is at 562.97nm. This is the 1000cm^{-1} peak.

$$1045cm^{-1} \cong \left(\frac{1}{532nm} - \frac{1}{561nm}\right)$$

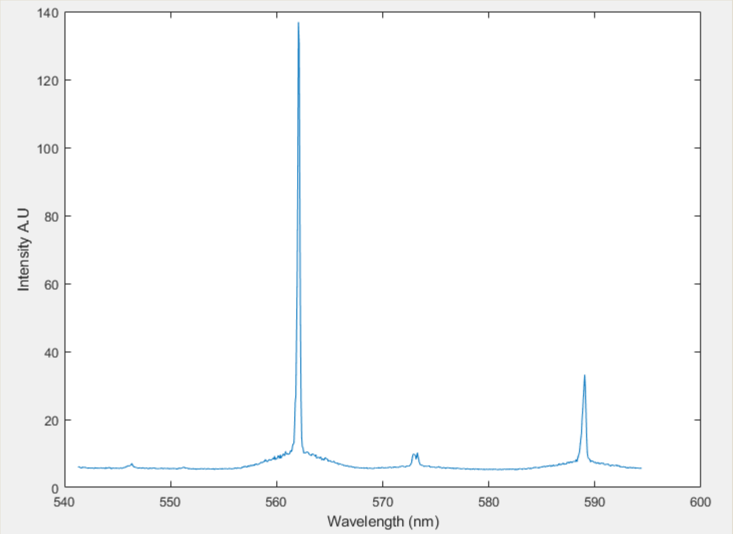
- The doublet at approximately 570nm is present, but for some reason other peak is not present.
- Peak at approximately 590 must be the peak sitting past 1500cm^{-1}. Gratings were tilted further in order to recalibrate; this may be part of the reason for the intensity of this peak to be larger.

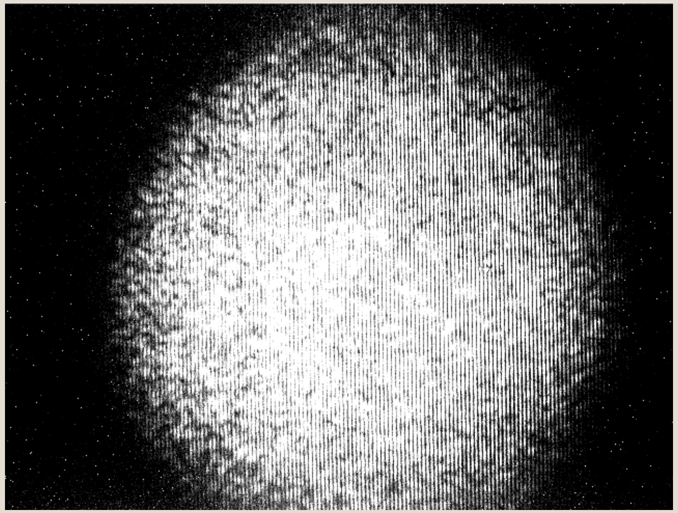
Measurements –Ammonium Nitrate



1750mg/ml

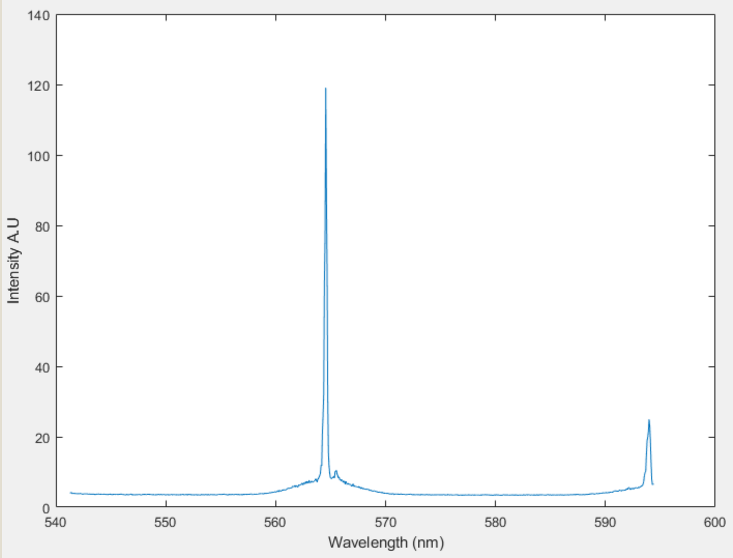
Exposure Time: 10 seconds





550mg/ml Concentration

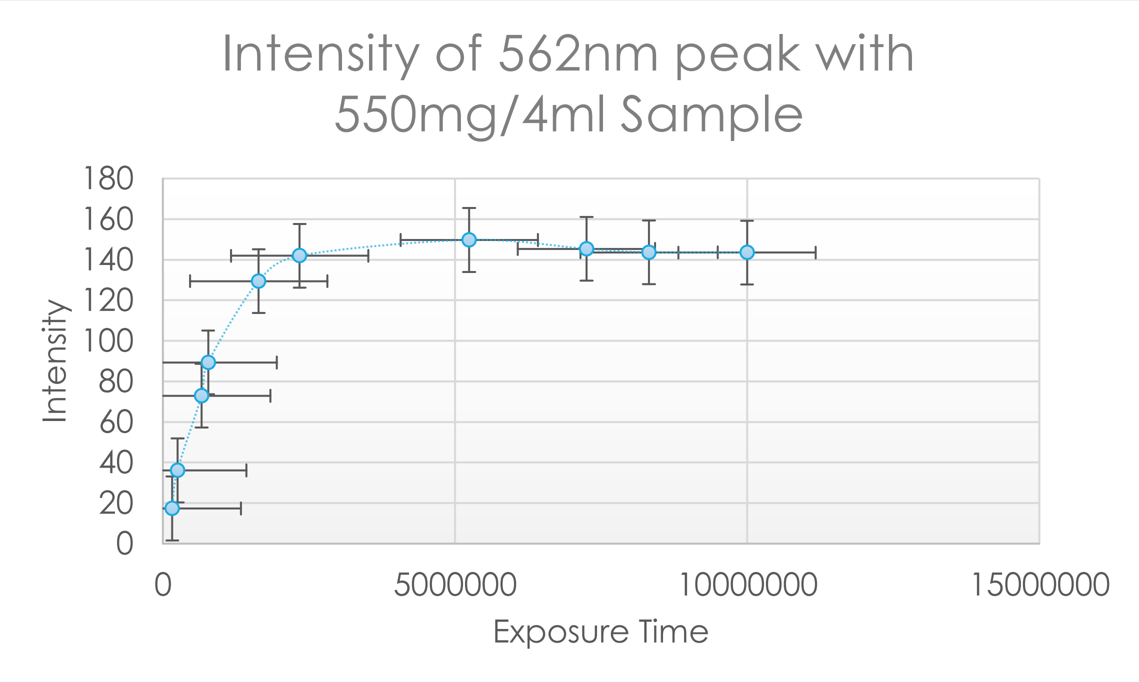
Exposure Time: 10 seconds



George McDonald

10 Measurements for Potassium Perchlorate

Concentration Level 2	
Exposure Time (us)	Intensity of 562nm peak
160233	17.3272
251473	36.1045
663573	72.9026
775381	89.304
1639053	129.431
2340773	141.9173
5242008	149.708
7250572	145.3213
8321082	143.6018
10000000	143.502

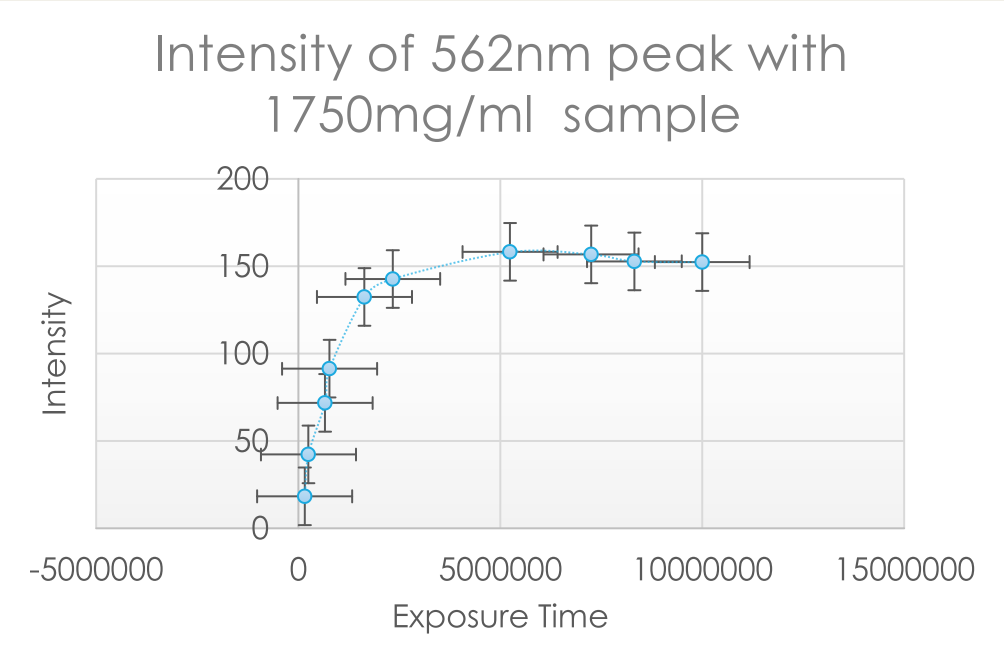


Average Intensity: 106.912

Julia Smith

10 Measurements for Potassium Perchlorate

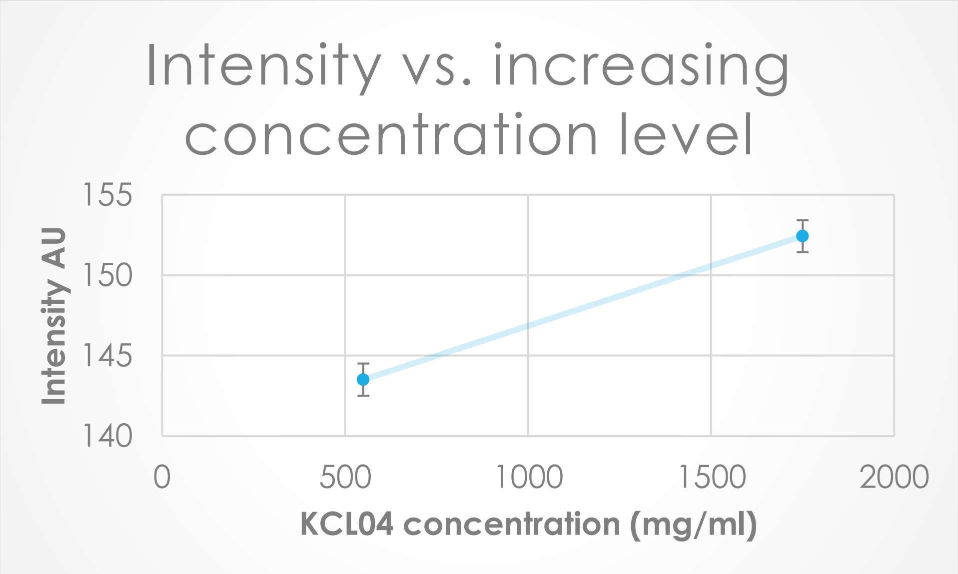
Concentration Level 1	
Exposure Time (us)	Intensity of 562nm peak
160233	18.3717
251473	42.314
663573	71.8034
775381	91.4056
1639053	132.477
2340773	142.814
5242008	158.23
7250572	156.81
8321082	152.8786
10000000	152.425



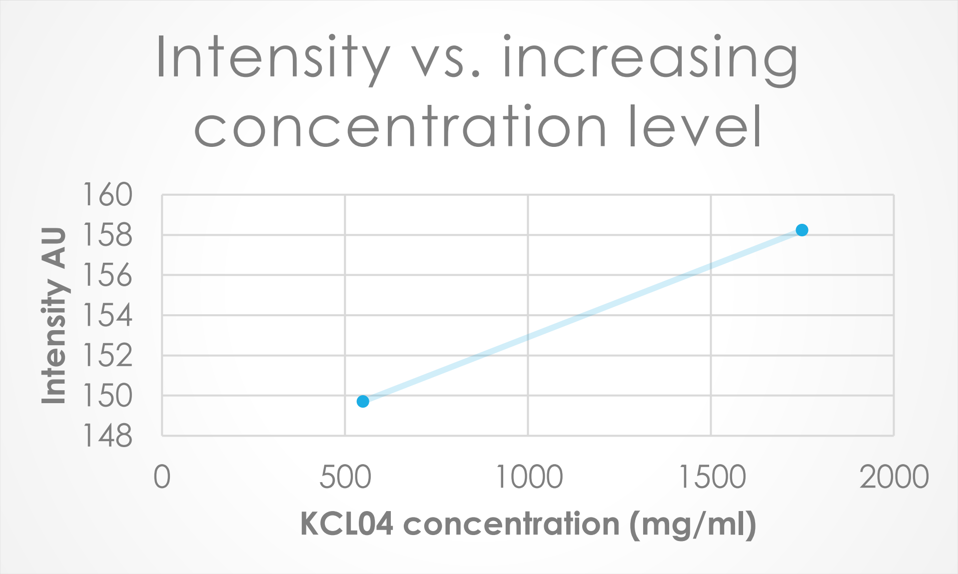
Average Intensity = 111.9529

Julia Smith

10 Measurements for Potassium Perchlorate



Exposure Time: 10s

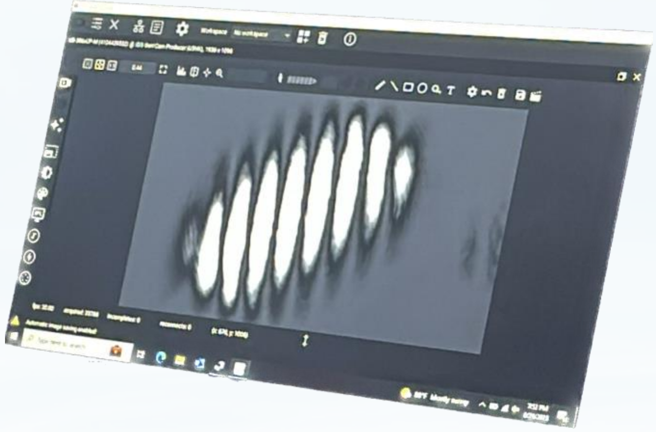


Exposure Time: 5.24s

George McDonald

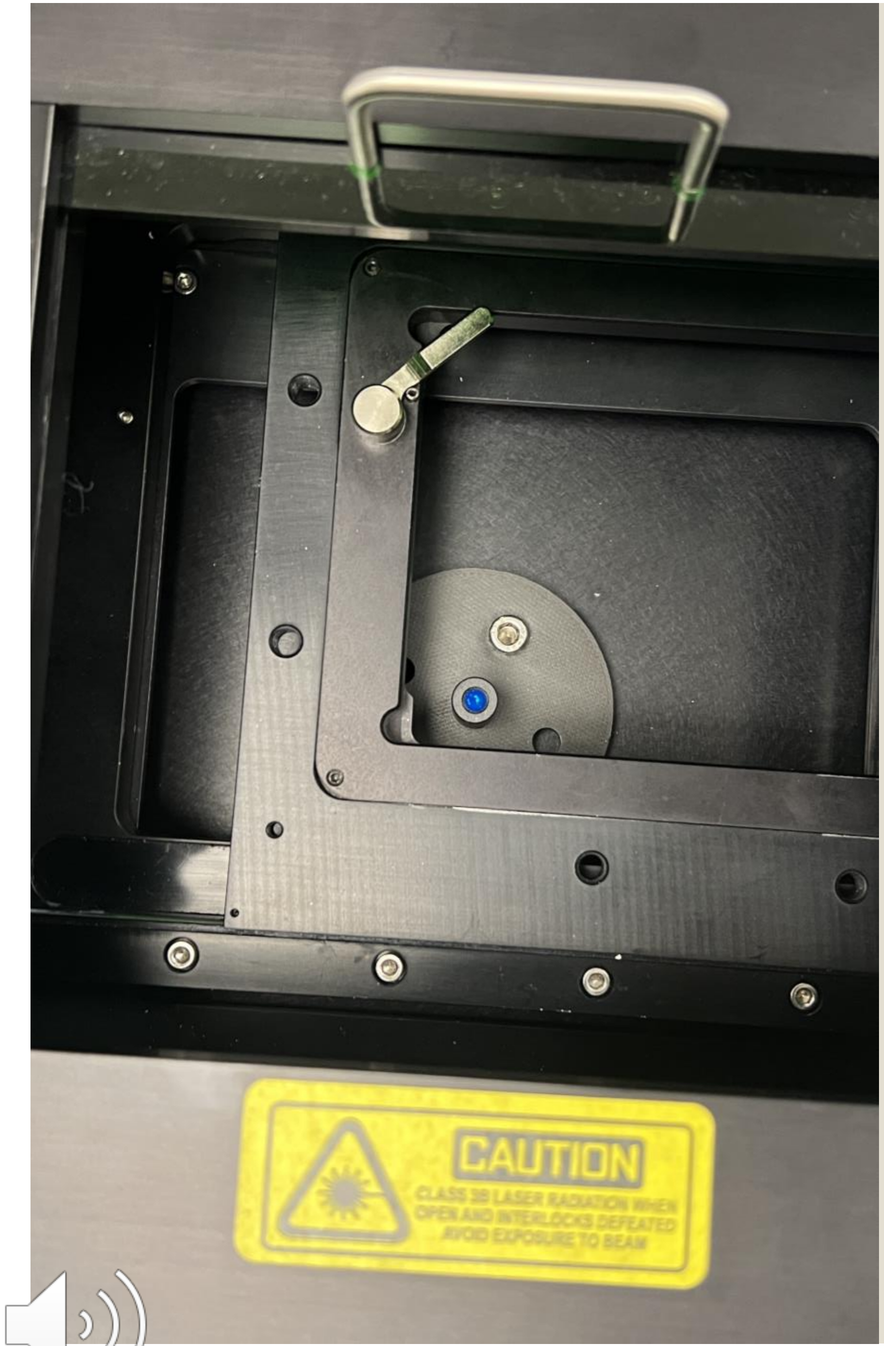
Optical Setbacks

Optical problems we ran into:



- **Problem :** 785nm laser was weak to have fringes be detected.
  - **Solution :** Found a new laser from Ocean Insight because it was strong.
- **Problem :** Gratings were not clean and had defects.
  - **Solution :** Got new grating for the spectrometer for better results.
- **Problem :** The spectrometer was very sensitive and had to keep re-aligning which led to poor resolution.
  - **Solution :** Put collars and more stable mounts on the optical breadboard.
- **Problem :** The camera that was bought initially was not efficient enough when we had 785 nm laser.
  - **Solution :** Used another camera that has a bigger sensing area and is more efficient in visible range. Switching lasers from 785nm to 532nm allowed us to operate in a spectral range where the frequency shifted signals could be picked up along with the corresponding fringes.

Julia Smith



Design Constraints and Standards – Optical

The biggest constraint was the laser that we are using for this project since it's a class 3 laser.

- The beam is hazardous to the eye and skin.

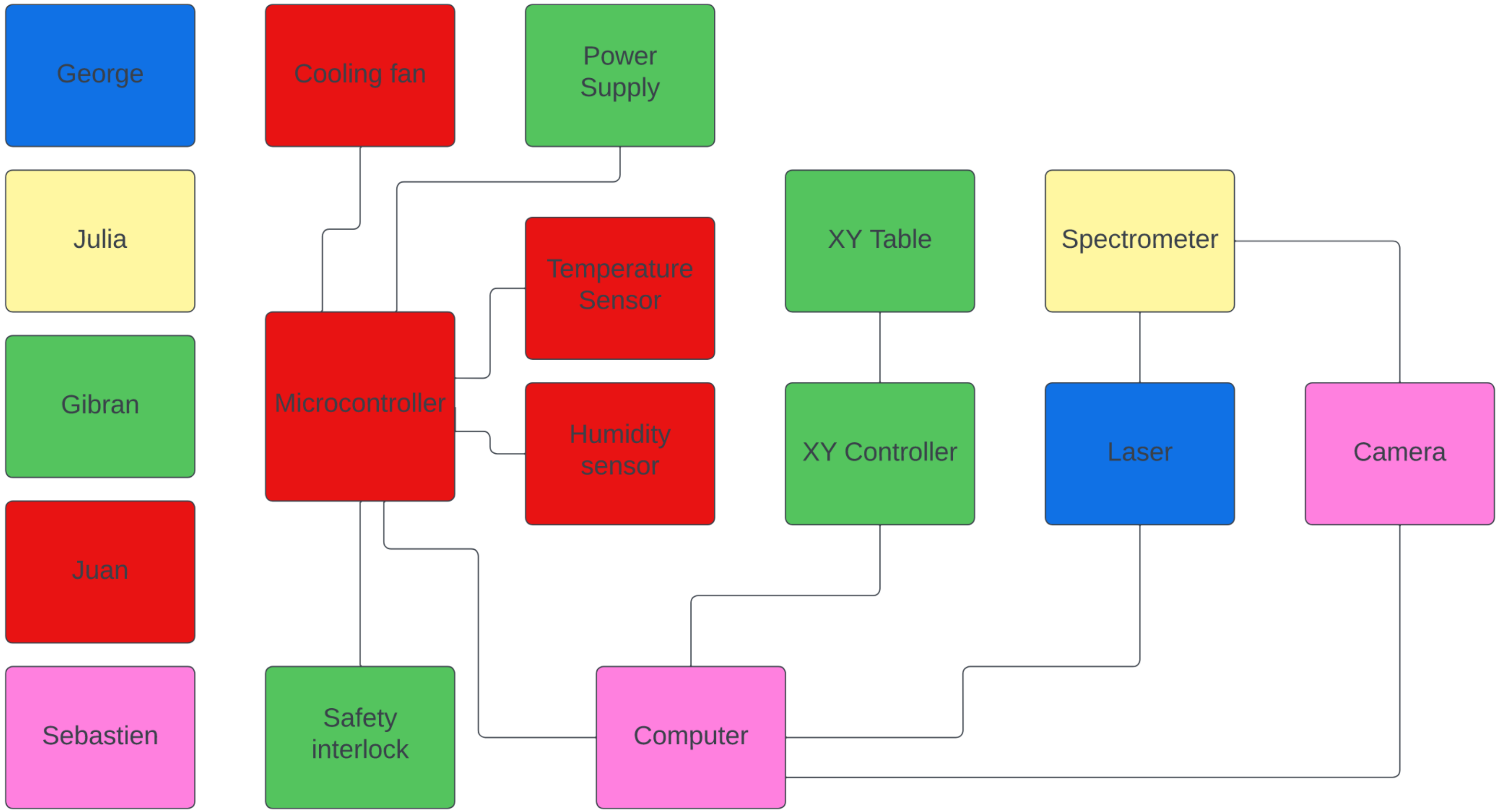
Another constraint was the chemicals we used while testing are flammable and can be harmful to the skin and eyes if not handled properly.

- Used a fume hood and gloves.

Julia Smith

Electrical Hardware & Software

Hardware Block Diagram



Gibran Khalil

Humidity/Temperature Factors

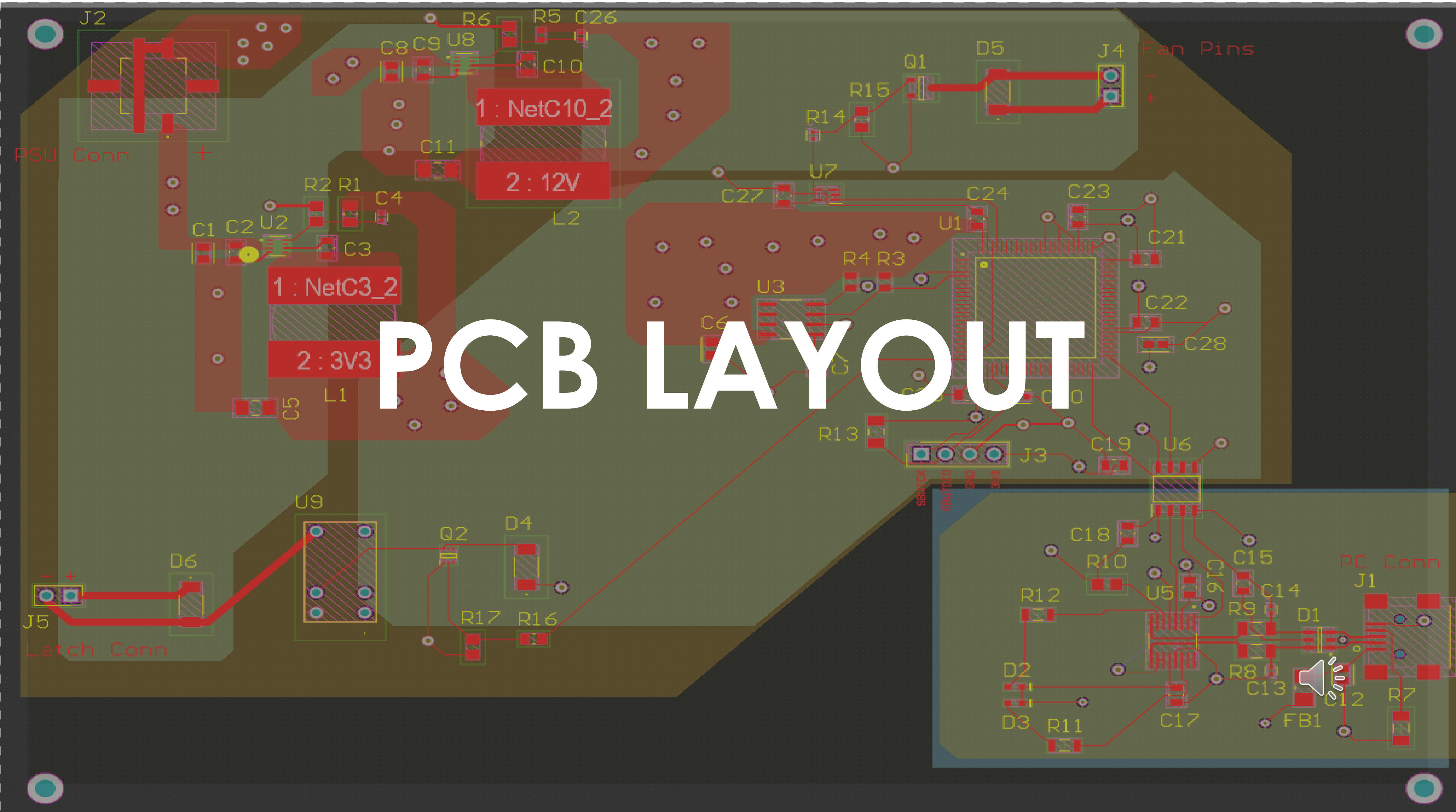
- Performance and accuracy of spectrometer.
- Water sampling
- Overall system ventilation/moisture
- I2C
- Fan to draw <500mA

Feature	SHT33-DIS-B2.5kS	SHT40-AD1F-R2	HIH6030-021-001
Voltage Rating	2.15-5.5V	1.08-3.3V	2.3-5.5V
Current Drawn	6mA-15mA	3.2mA-5mA	6.5mA
Size	2.5mm x 2.5mm	1.5mm x 1.5mm	SOIC-8
Pins	8	4	8
Price	$9.60	$3.12	$12.5
Diff. Description	DFN Package	Small functionality	SOIC-8 Package

MODEL	input voltage rated (Vdc)	input voltage range (Vdc)	input current[1] max (A)	input power[1] max (W)	rated speed[1] typ (RPM±10%)	airflow[2] (CFM)	static pressure[3] (inch H_2O)	noise[4] typ (dBA)
CFM-8025BG-140-396	12	10.8~13.2	0.27	3.24	4,000	41.40	0.27	39.6
CFM-8025BG-150-444	12	10.8~13.2	0.35	4.20	5,000	51.74	0.43	44.5

Juan Restrepo Diaz

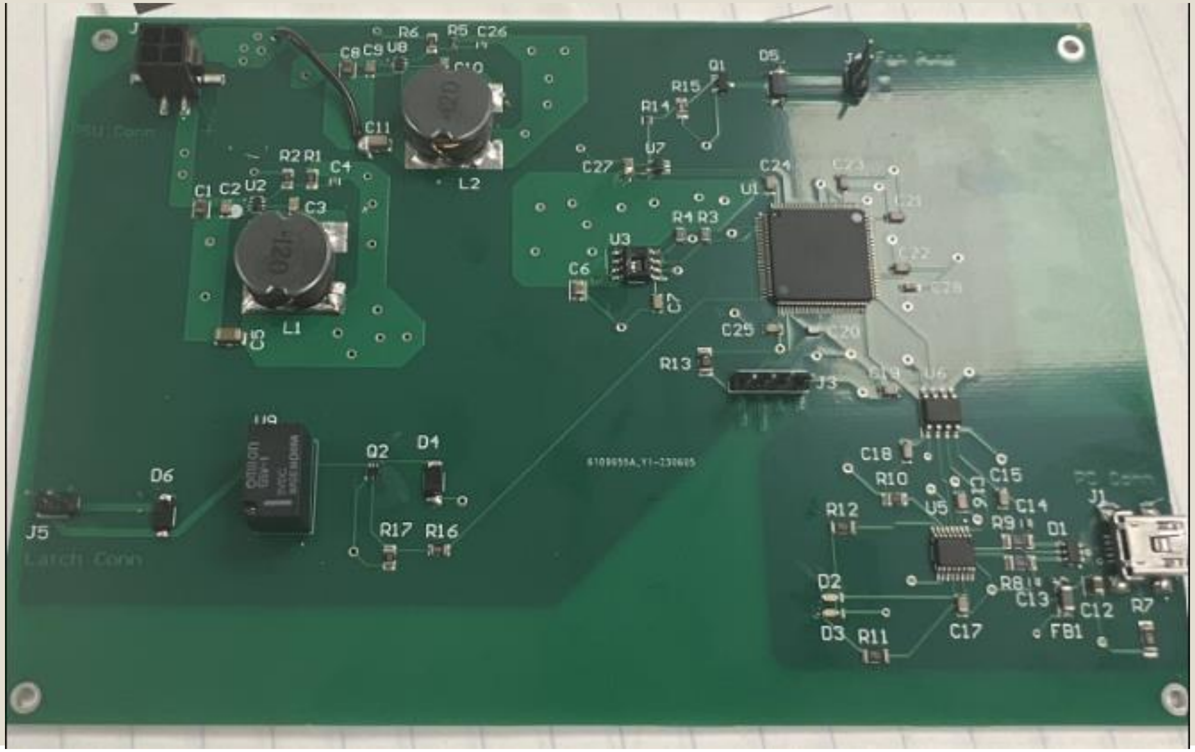
PCB LAYOUT

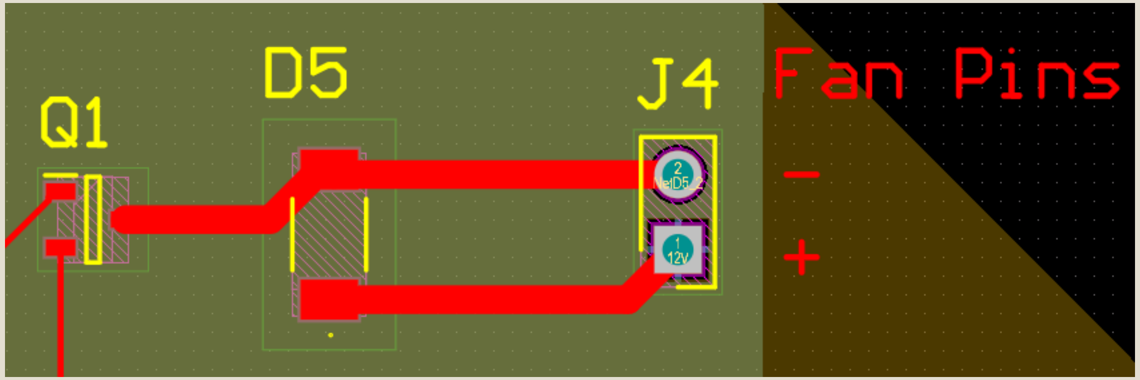


J2
PSU Conn
+
R6
R5
C26
C8
C9
U8
C10
1 : NetC10_2
2 : 12V
L2
C11
Q1
D5
J4
Fan Pins
-
+
R15
R14
U7
C27
C24
C23
U1
C21
R4
R3
U3
C6
C22
C28
R2
R1
C4
C1
C2
U2
C3
1 : NetC3_2
2 : 3V3
L1
C5
R13
J3
C19
U6
U9
Q2
D4
D6
J5
- +
Latch Conn
R17
R16
C18
R10
C15
PC Conn
J1
R12
U5
C14
R9
D1
D2
R8
C13
D3
R11
C17
FB1
C12
R7

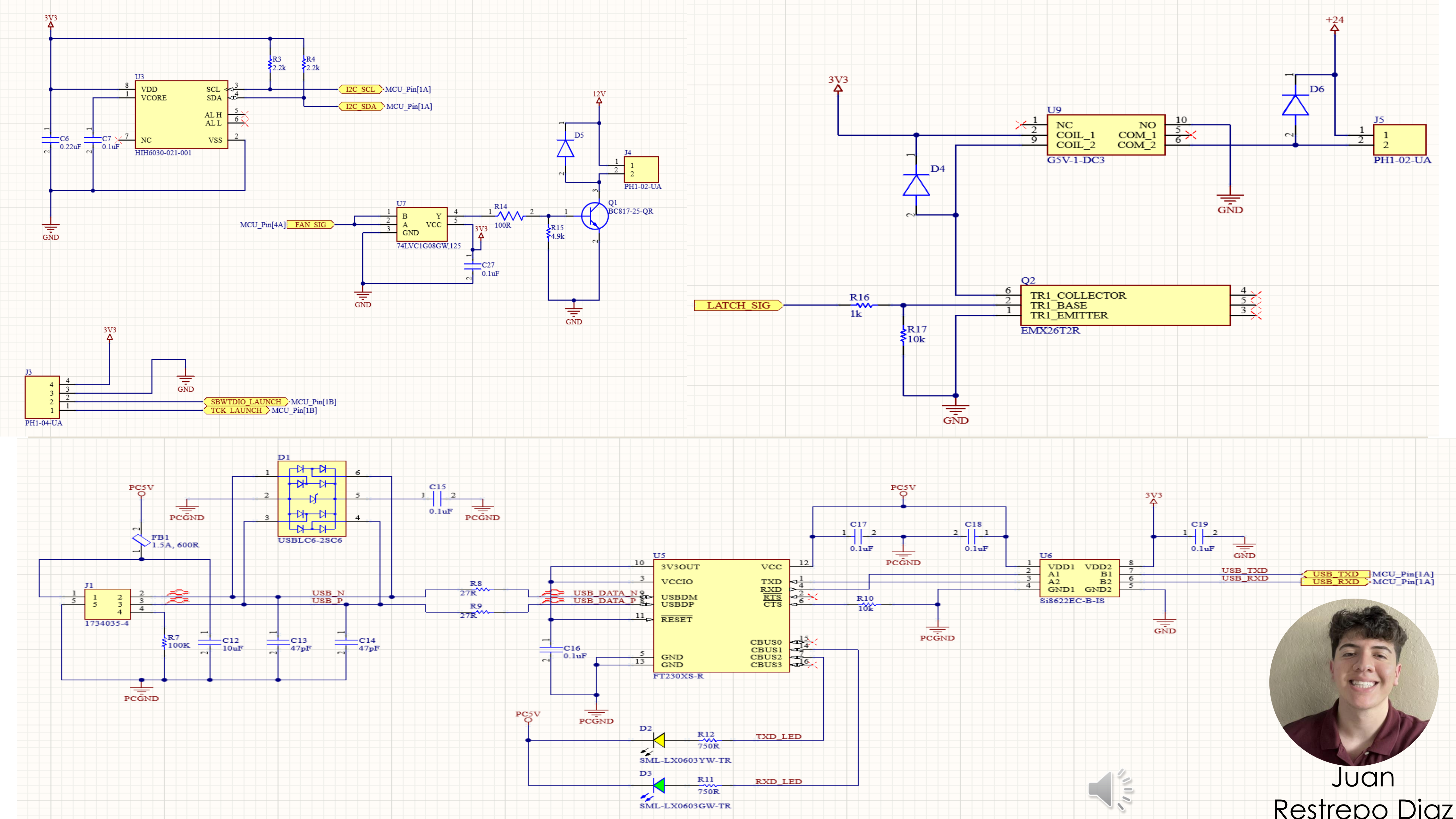
PCB Layout & Schematics

- Altium Designer
- Manufacturer Recommendations
- Challenge, Industry





Juan Restrepo Diaz

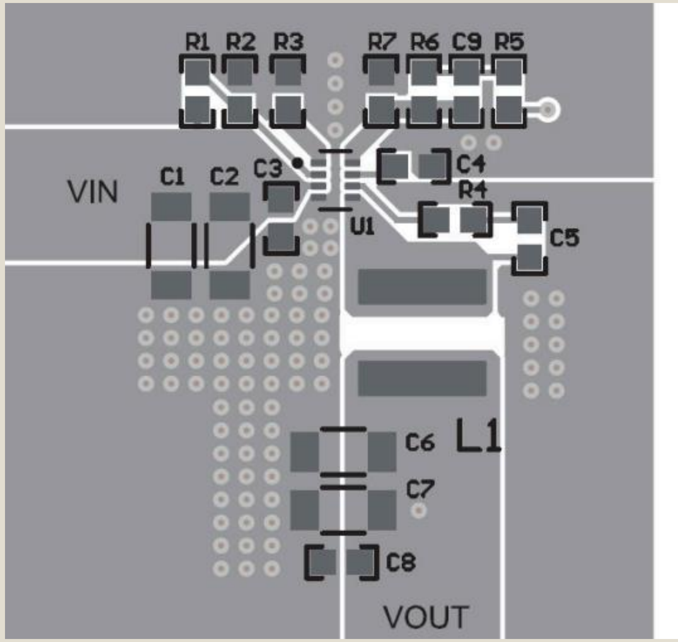


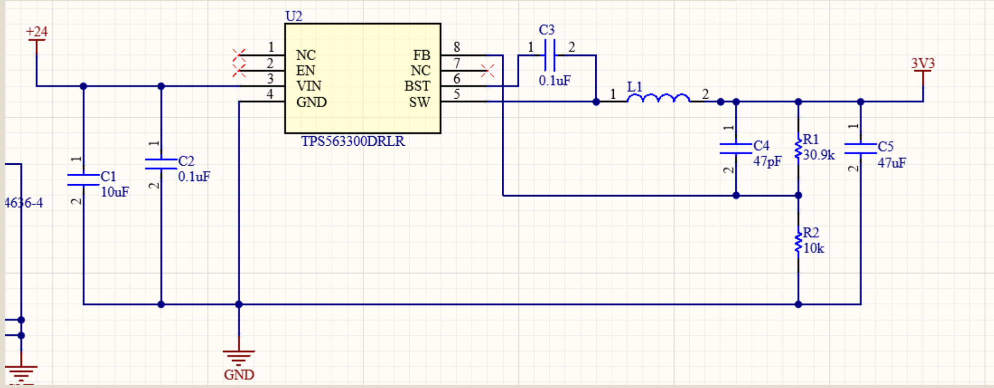
Juan Restrepo Diaz

Power Distribution

- 24V Power Supply
- TI WEBench
- Buck Converters into 12V and 3V3 rails
- Current loop layout per manufacturer specifications

Feature	TPS563300DRLR	LM317MDT-TR	MAX25302BATD/V+
Voltage Rating	3.8V – 28V	4.2V – 40V	1.7V – 5.5V
Max Current Output	3A	1.5 A	2A
Voltage output	800 mV to 22 V	1.2 V to 37 V	600 mV to 5 V
Size	1.6-mm × 2.1-mm	2.4mm x 6mm	SOIC-8
Pins	8	4	14
Price	$1.70	$0.90	$1.94
Reasoning	Buck converter, TI webench simplicity	Outdated component	TDFN package, Does not meet new output requirements

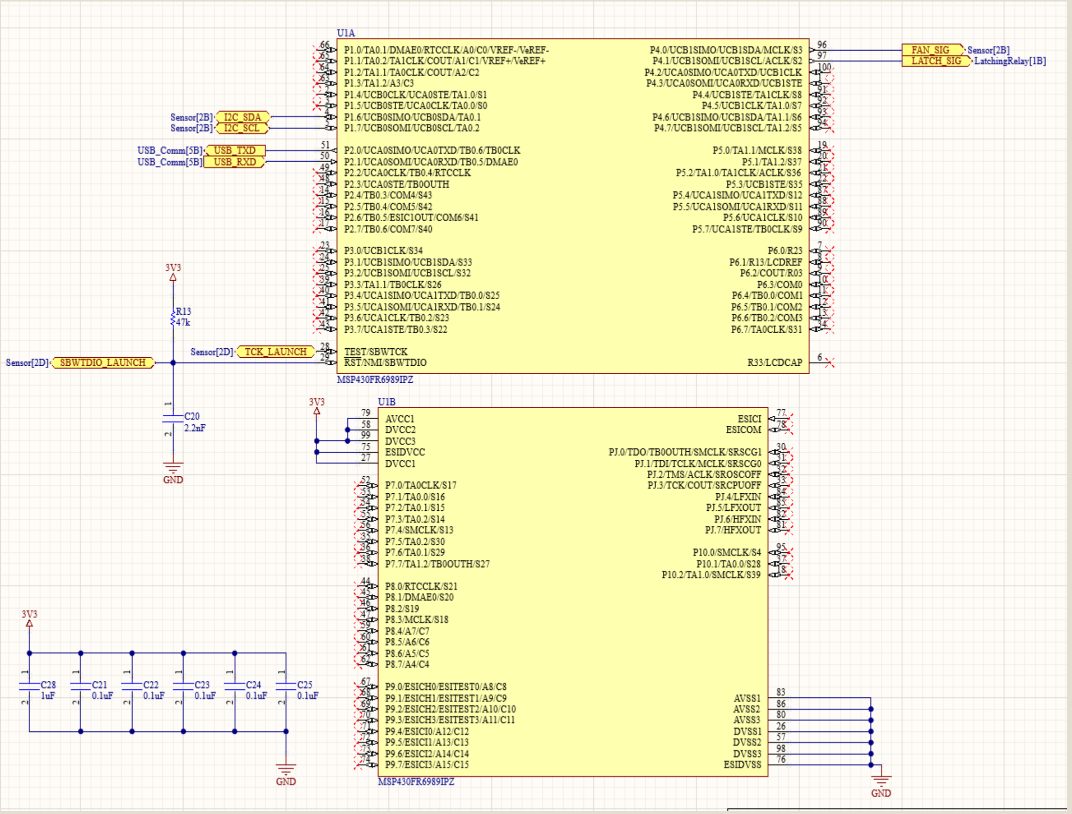




Juan Restrepo Diaz

MCU/ Programming

- Spy-by-Wire technology
- Logic gates for signal reinforcing
- MSP430EXP Development Board

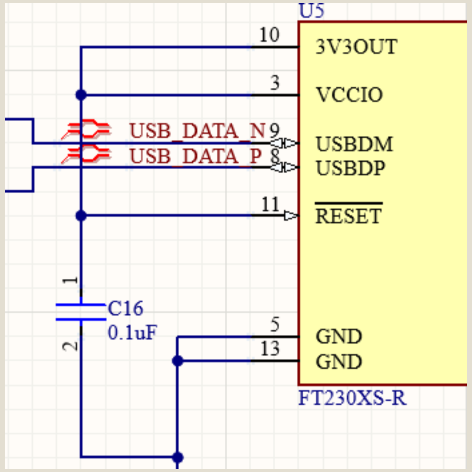


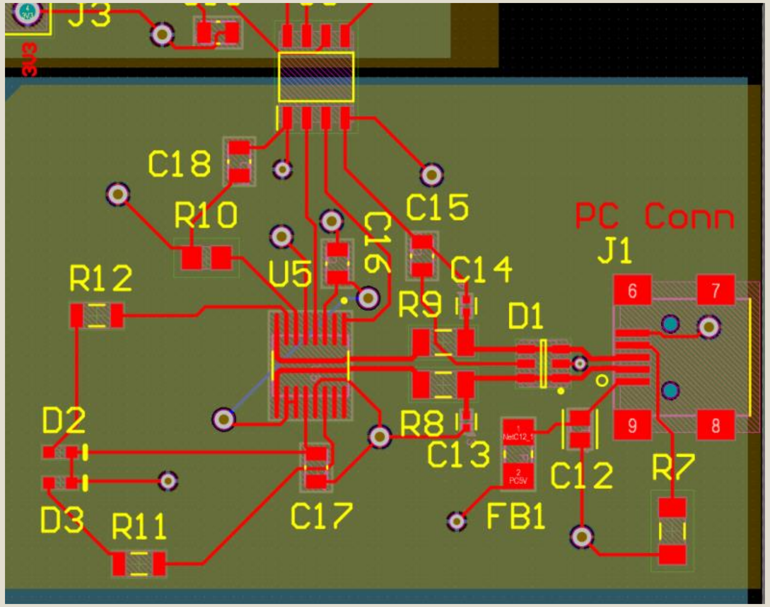
Feature	MSP430FR6989	STM32G431C6T6
Voltage Rating	1.8-3.6V	1.7-3.6V
GPIO Pins	74	38
Protocols supported	I2C, SPI, UART	I2C, SPI, UART, USART, USB
Pins	100	48
Price	$11.2	$7.1
Reasoning	CCS, familiar with programming. Spy-By-Wire programming through Dev board	STMCubeProg

Juan Restrepo Diaz

USB Layout

- Differential Pairs
- UART to USB connection with PC
- Isolation
- LEDs
- Trace specifications





Juan
Restrepo Diaz

Safety Interlocks

Safety interlock on enclosure.

Laser is in operation and enclosure is closed to prevent eye injuries.

Operation cannot be interrupted by user.

Gibran Khalil

Safety lock specifications

	Banner Engineering SI-LS42DMMGF	IDEC HS1L	Omron Automation and Safety TL4019
Max Holding Force(Locked)	1500N	3000N	1200N
Operating Temperature Range	-20C to 70C	-20C to 55C	
Power Consumption	4.4W	4.8W	8W
Operating Voltage	110/230VAC or 24VAC/VDC	24VDC	24VAC/24VDC Or 110VAC
Switch Operations per hour.	600	900	
Maximum Actuator Speed	0.5m/s	1m/s	0.33m/s
Mechanical Life operations	1000000	1000000	1000000
Price	~426$	~200$	~552$

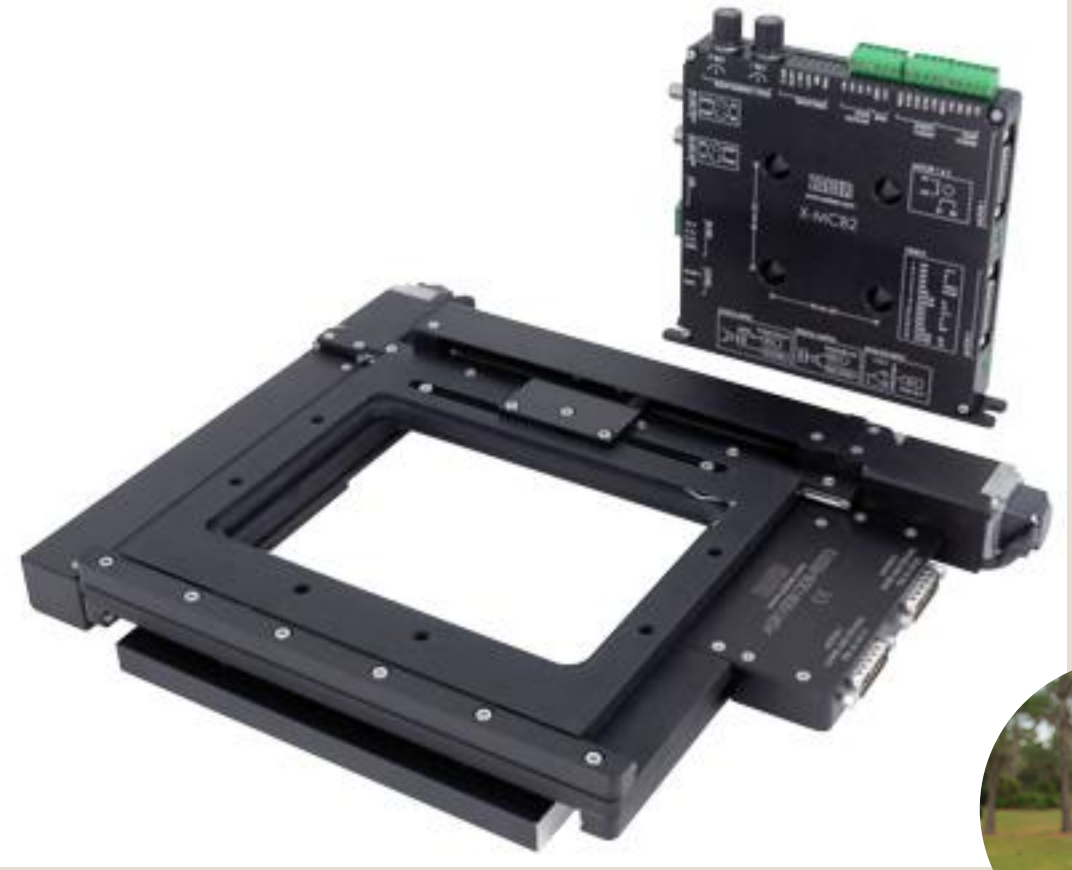
Gibran Khalil

XY Table

Allows usage of well plate

Multiple samples allowed at once for mass data gathering

High resolution allows for accurate laser usage



Gibran Khalil

XY table specifications

XY Table Model	ZABER ASR	PI L-731	MOXY-01-100-100
Controller compatibility.	XMCC With autodetect	None included manufacturer has recommended list	None included or sold by manufacturer
Travel Range	100x120	205x205	100x100
Resolution	0.15625um	1nm	1.25um
Motor type	Stepper (2 phase)	DC Motor	NEMA17 Stepper motor
Max Speed	85mm/s	50m/s-90mms	20mm/s
Price	Order Dependent	Order Dependent	2739$
Operating Temperature range	0C to 50C	5C to 40C	Unknown

Gibran Khalil

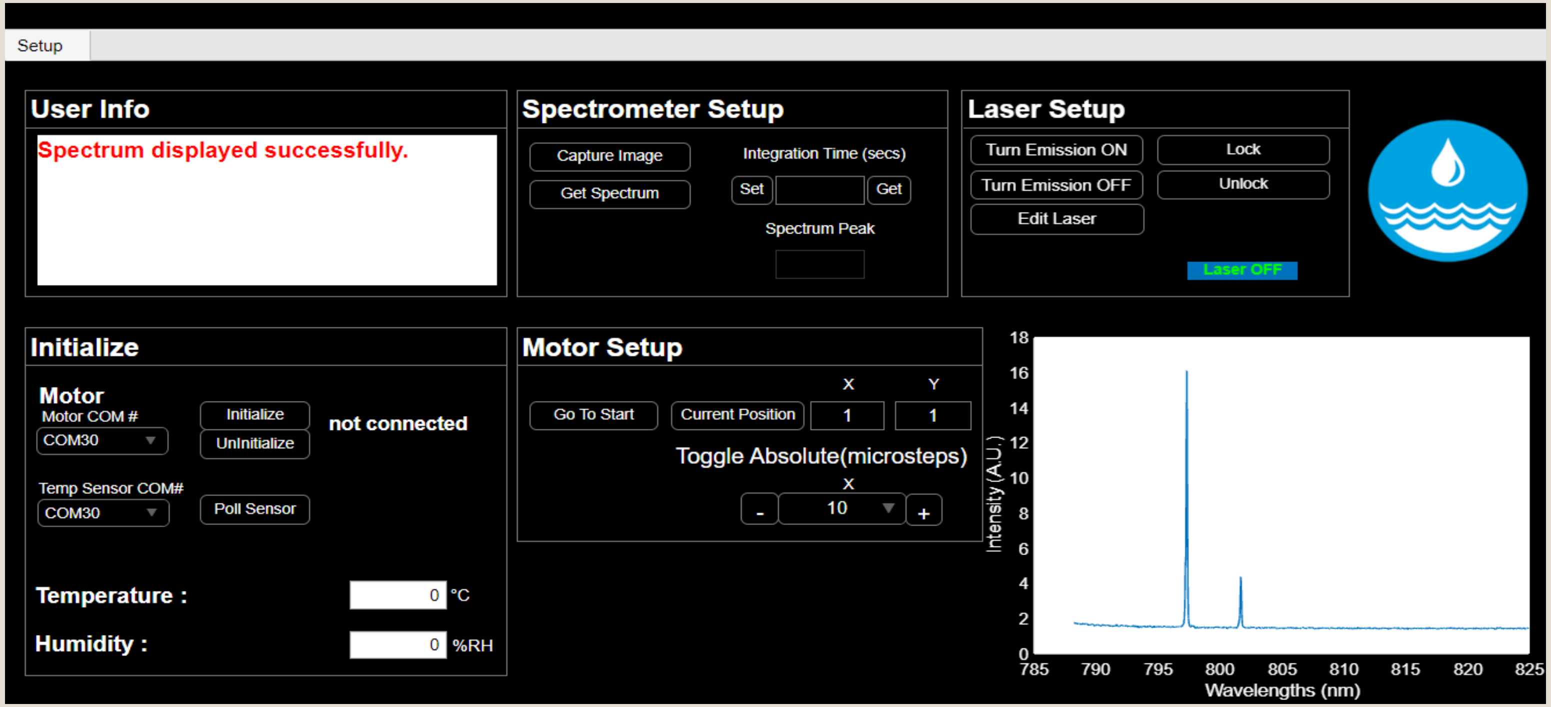
Computer Specifications

- MATLAB and supporting libraries have specifications to be able to run
- Large storage is required to store all the data that will be used to perform calculations.
- RAM is an important aspect to be able to perform the calculations themselves.

	Latte Panda	Dell XPS 13 9315	ASUS ZenBook Q526FA
Processor	Intel Atom x5-Z8350	Intel Core i5-1230U	Intel Core i7-8565U
Number of Cores	4	8	4
Storage Type	HDD	HDD	SSD-HDD Hybrid
Storage Capacity	64 GB	256 GB	1128 GB
RAM	4 GB	8 GB	16 GB
Operating System	Windows 10	Windows 11	Windows 11
System Type	64-bit	64-bit	64-bit

Sebastien Jouhaud

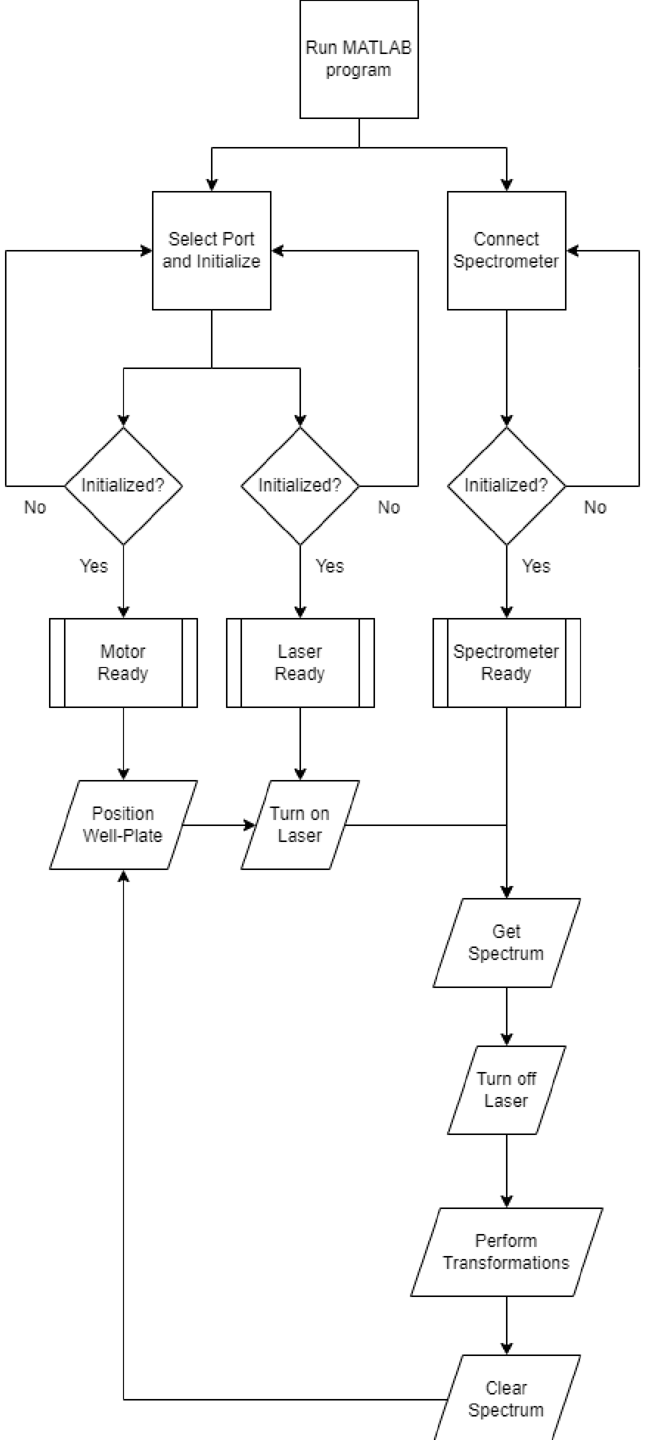
Graphical User Interface



- The GUI is used to control the system as a whole and allows the user to make the adjustments available to them as they see fit.
- Most of the features in the GUI require user input in order to make it as user friendly as possible.
- Initialization and control of the various components is made through the GUI.
- Motor positioning, laser state, and safety features are controlled through the GUI.

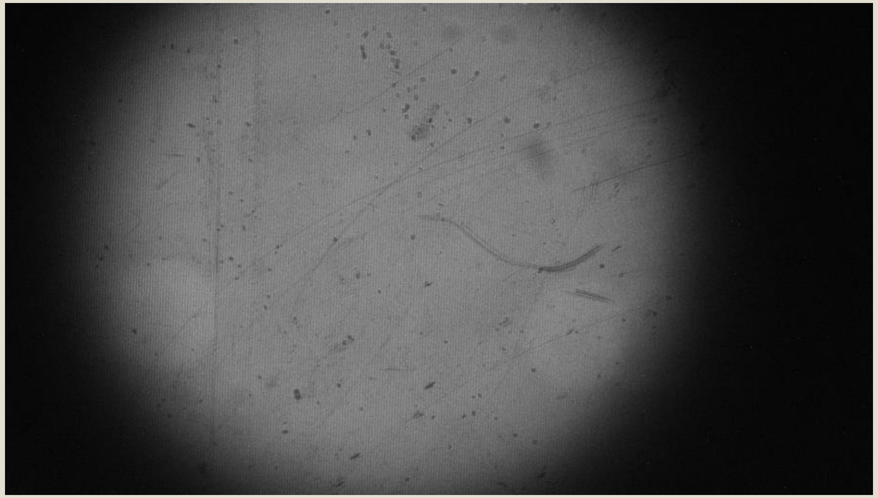
Sebastien Jouhaud

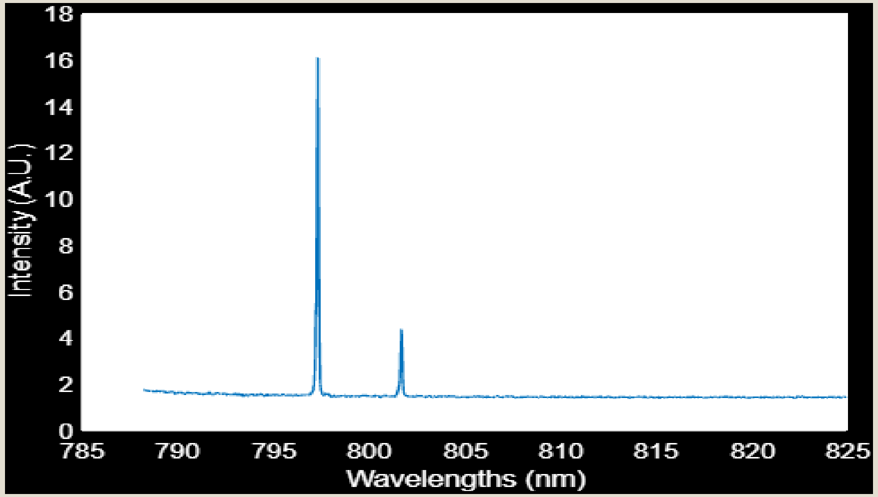
Software Block Diagram



Sebastien Jouhaud

Fourier Transformation





- Camera takes multiple pictures of the fringes.
- The IDS Eye camera communicates with MATLAB in order to convert these images into mathematical matrices.
- A Fourier transform is then applied to the numerical matrix, and a graph is created.
- This graph has peaks at certain wavelengths that describe the chemical makeup of the sample.

Sebastien Jouhaud

Budget

ITEM	QUANTITY	PRICE ESTIMATE
Laser	1	Acquired
Gratings	2	~$160
Lens	3-4	~$260
CCD	1	$700
Motor translation stage	1	$1495
XY Table with additional components	1	$5876
Polarized beam splitter	1	$880
Power Source	1	$10
Custom PCB	1-2	$80
Custom Enclosure	1	TBD
Microcontroller	1	$15
Connectors	3	$10
Misc. Components	TBD	$30
TOTAL	N/A	~$9516

Thanks for listening!

Q&A?