



Developing Python Interface and Autonomous Scanning for FTMW Spectrometer

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Research Investigations & Objectives

- Developing overarching Python software controlling Tektronix oscilloscope, Zaber actuator, Stanford Research delay generator, Valon synthesizer, and other components
- Autonomous scanning capabilities for positioning actuator based on Fourier transform of obtained waveforms in Python
- Synchronous and simultaneous control and operation of novel FTMW spectrometer via GUI

Background

- FTMW (Fourier transform microwave) spectroscopy measures molecular transitions between quantized rotational energy levels.
- FTMW spectroscopy, when combined with supersonic molecular beams, offers a near collision-free environment to investigate fundamental properties and dynamics of Van der Waal complexes, short-lived intermediates, radicals, combustion/pyrolysis products, etc.
- Diluted analyte is pulsed into a vacuum and excited by short (<1 us) microwave pulses to record rotational spectra
- FTMW spectrometer designed by Dr. Gurusinghe research lab combines Cavity and Chirped pulse FTMW setups in a novel L-shaped design (**Figure 1**) with integrated instruments described in **Table 1/Figure 2**
- Implementation of Python overarching software allows for the development of a multitude of tools through simultaneous instrumentation control on top of ease of spectrometer use

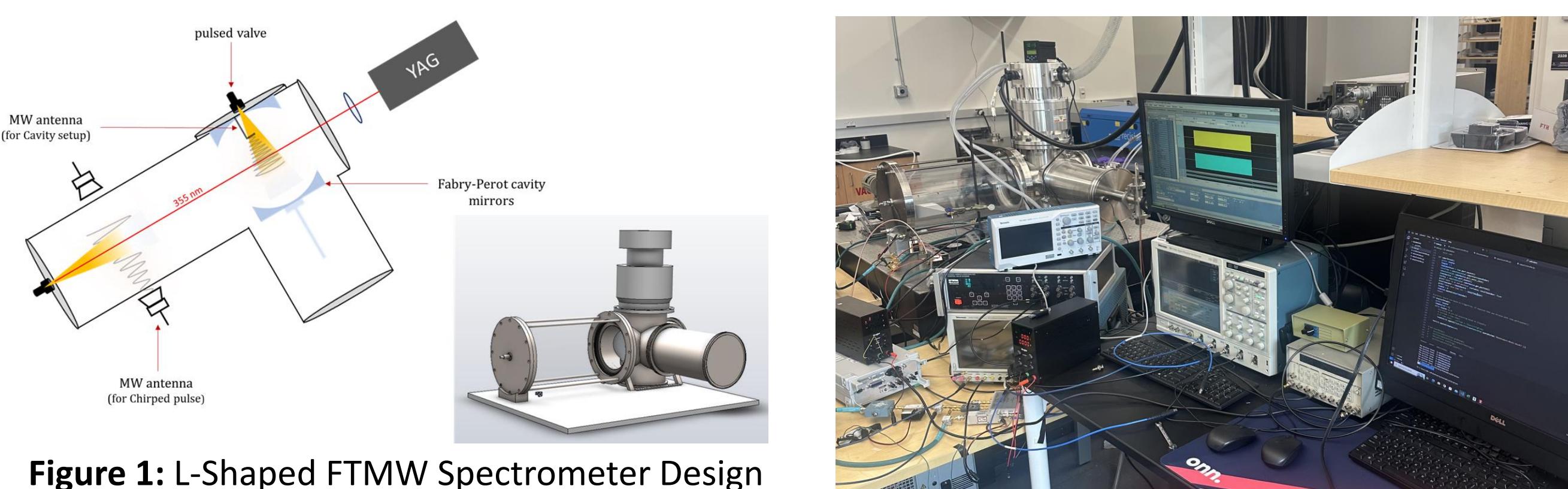


Figure 1: L-Shaped FTMW Spectrometer Design

Instrument	Type	Purpose
Tektronix DPO7354	Oscilloscope	Data acquisition
Zaber XNA08A25-E09	Actuator	Fabry-Perot cavity tuning
SRS DG535	Delay generator	Triggering
Valon 5019	Synthesizer	Generate signal
Tektronix AWG7102	Waveform Generator	Generate Signal

Table 1: Main Instruments (red controlled by software)

Instrument Control & Design

- Microwave pulses are generated using AWG and Valon synthesizers and sent to the MW cavity
- Pulse rate dictated by the delay generator
- Cavity length is dictated by the mirror that Zaber actuator positions
- Collected free induction decay signals are routed to the oscilloscope for signal averaging and Fourier transformation

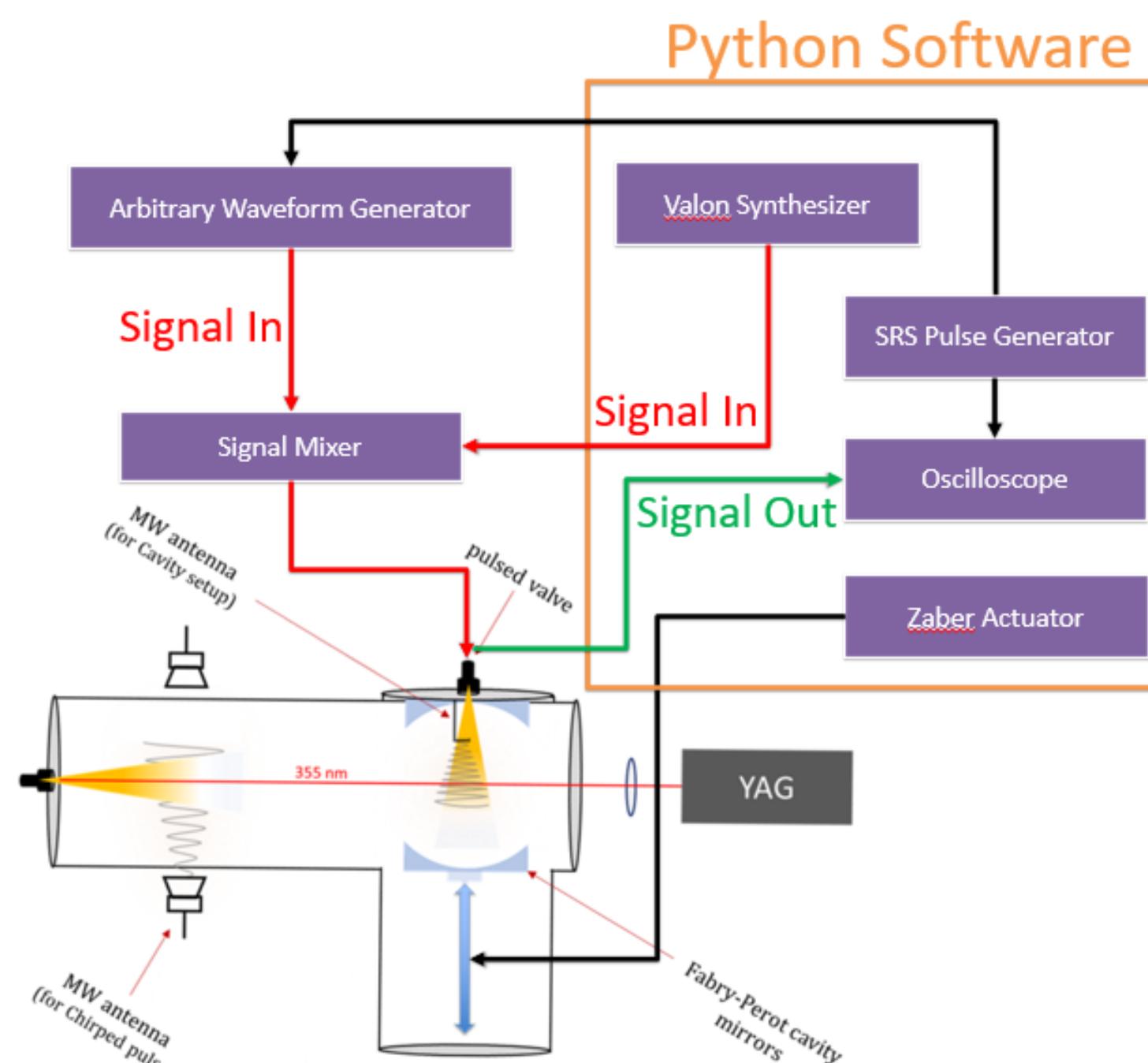
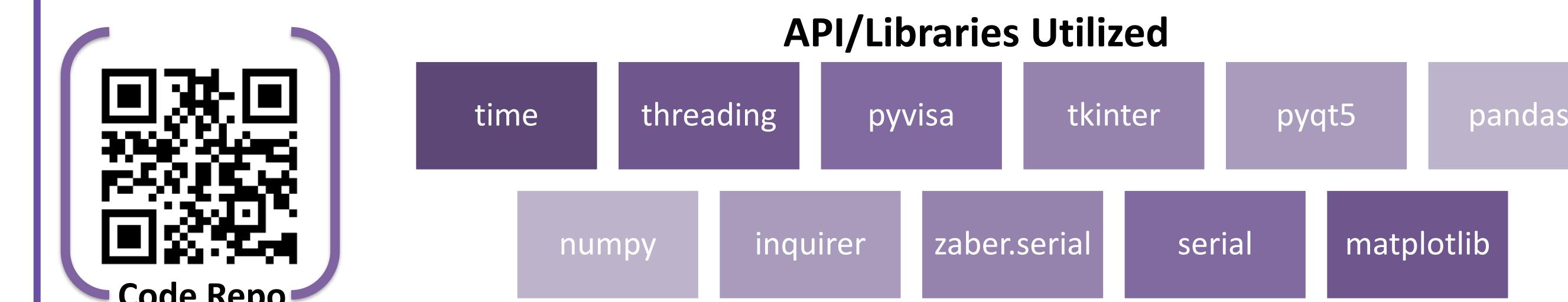


Figure 2: Spectrometer and Software Control Design

Software Design



- GPIB connected oscilloscope handled as pyVISA resource
- USB connected actuator handled as AsciiSerial device
- USB connected synthesizer handled as serial class
- GPIB connected pulse generator handled as pyVISA resource
- Binary/Ascii commands issued to initialize, program settings, and receive real time data
- GUI shell established via Tkinter and PyQt5 while live plotting done via matplotlib
- Threading initialized to receive oscilloscope data (~450 data pt. per second) while handling GUI shell and controlling other instruments according to data output, such as actuator position during calibration
- Ensuring synchronization of position data vs. intensity data handled via time modules to within ~ ±0.007 seconds accuracy as well as optimization via perf_counter()
- Numpy for N-dimensional arrays, Pandas for ease of data analysis
- Scanning handled via Python script coordinating instruments

Scanning Results/Conclusions

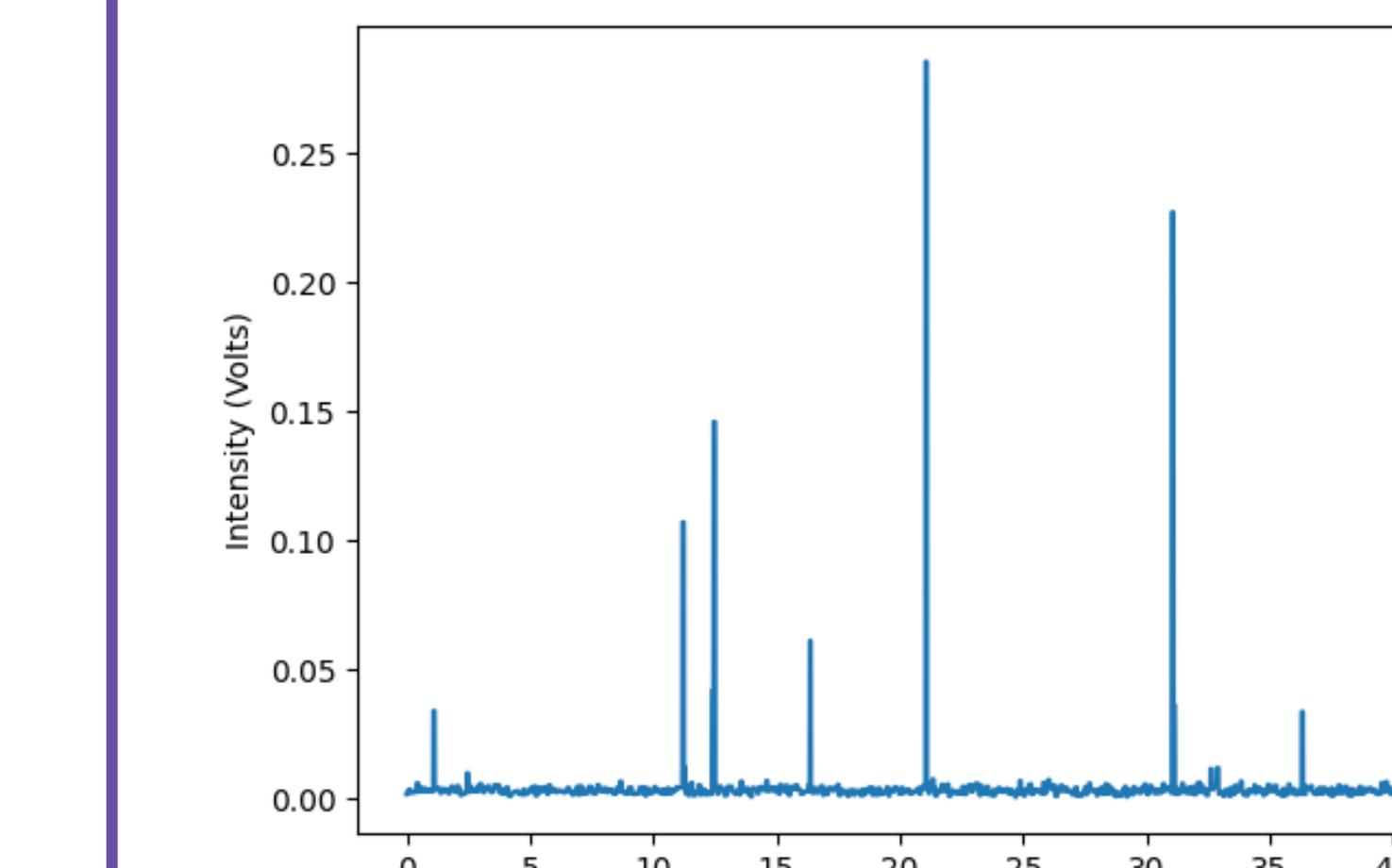


Figure 3: Calibration at 15,491.6451 MHz from 0 – 40mm

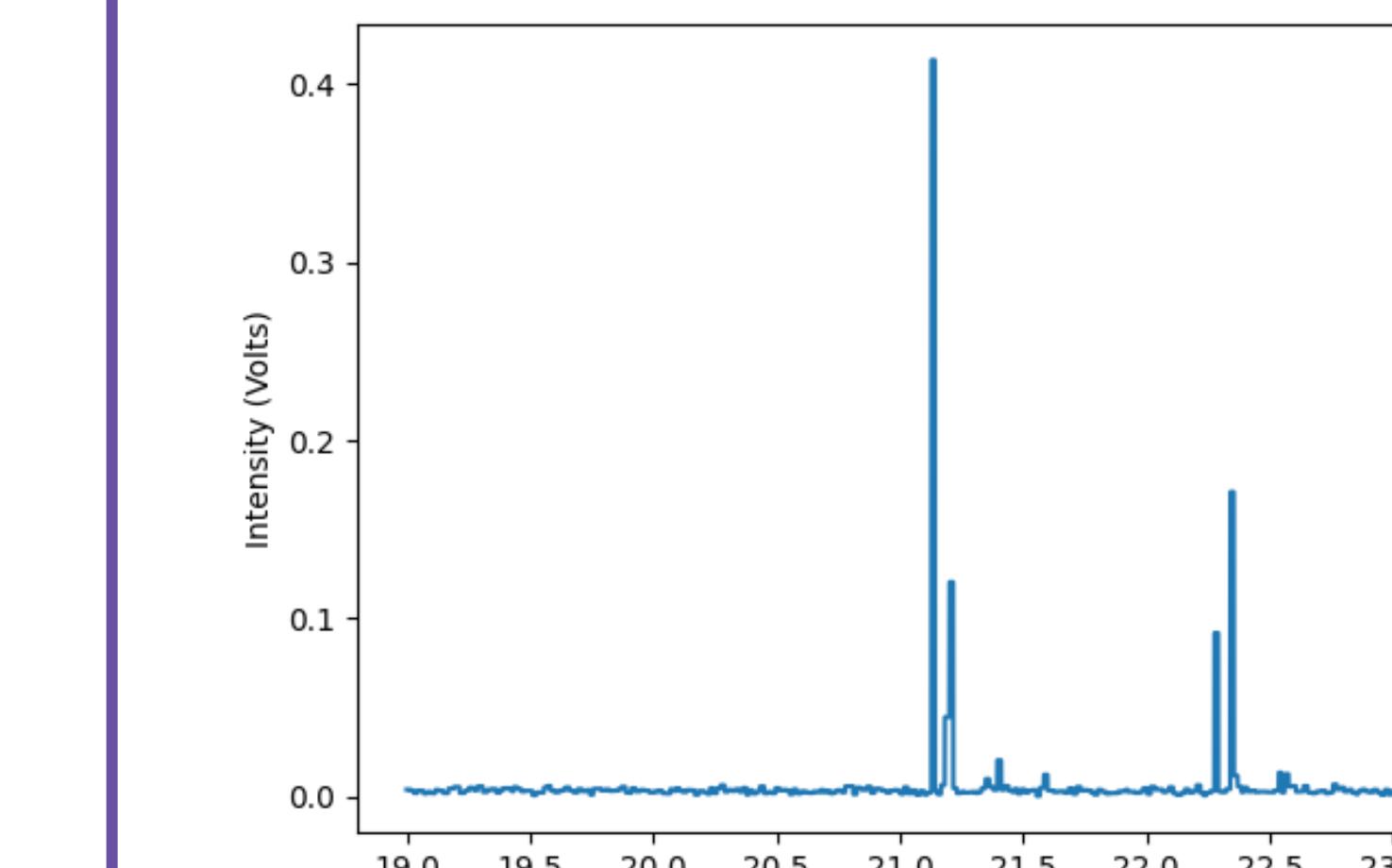


Figure 4: Calibration at 15,491.6451 MHz from 19 – 23mm

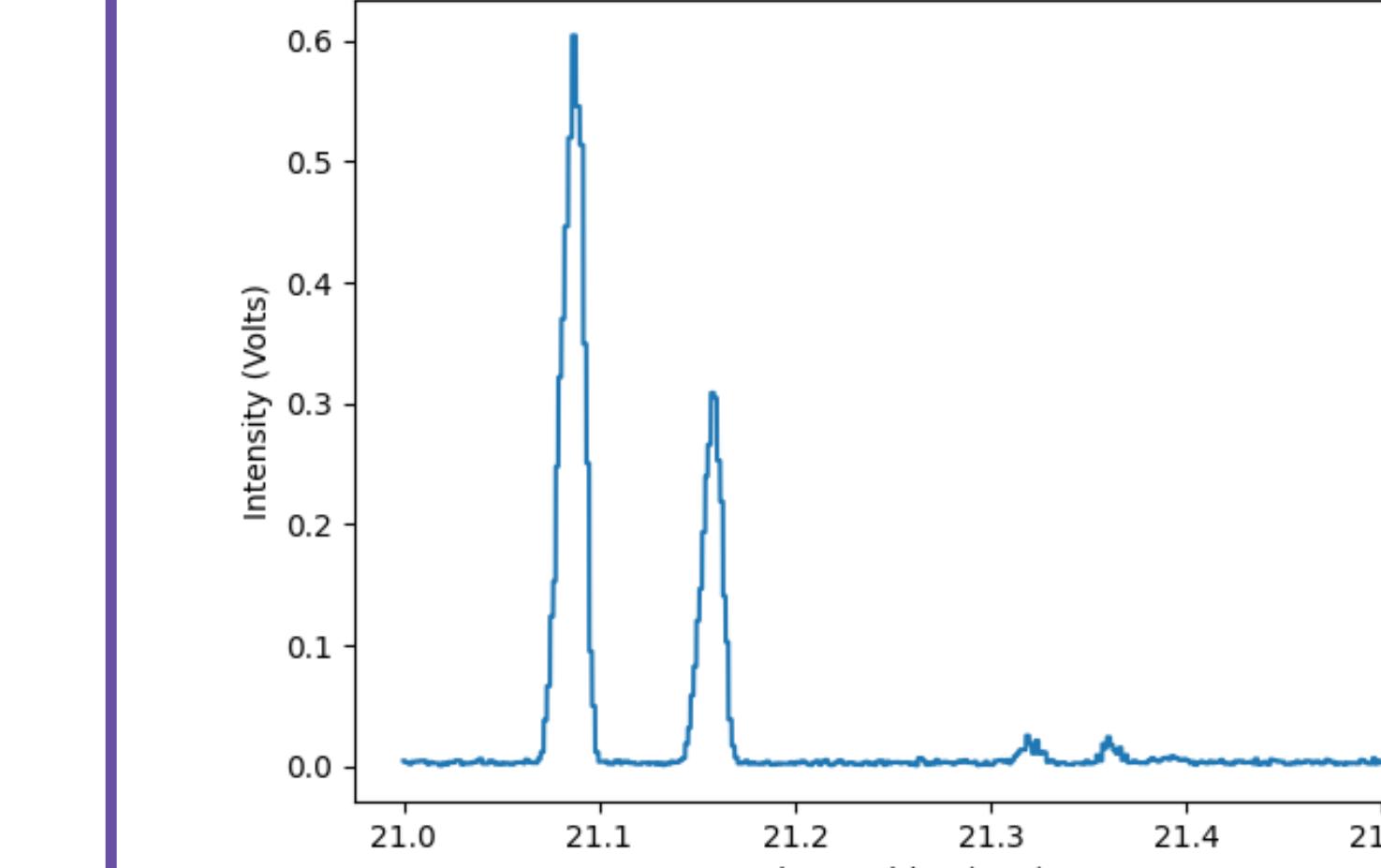


Figure 5: Calibration at 15,491.6451 MHz from 21.0 – 21.5mm

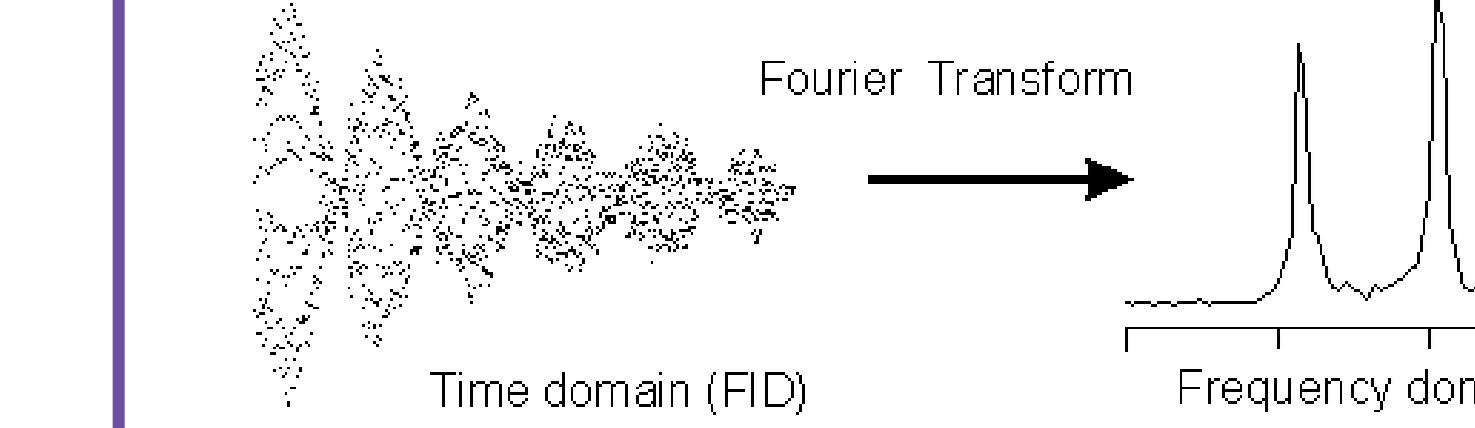


Figure 6: Fourier Transform of a Waveform

- Cavity tuning is fully handled by Python software
- For autonomous tuning, waveforms are generated via AWG/synthesizer on initialization of internal trigger by delay generator
- Determines ideal cavity length for a particular frequency for MW experiments
- Maximum is found with ±0.001 mm accuracy by continuing to refine actuator scan range limits and max actuator velocity
- Mirror actuator position is then fixed in the optimal position for experimentation
- Synthesizer frequency increased for the next run

```

9 v def initializeValon(port):
10   global valonConnect
11
12   #Creating class of valonConnection
13   class VSerialPort(serial.Serial):
14     def __init__(self, portParam = None):
15       serial.Serial.__init__(self)
16
17       self.baudrate = 9600
18       self.timeout = 1
19       self.port = port_name
20       self.open()
21       self.setDTR(False)
22       self.flushInput()
23       self.write([0x01])
24       self.write([0x02])
25       response_bytes = self.read(1024) #total bytes expected back from return
26       print(response_bytes)
27       #Mode (continuous wave)
28       print("-----")
29       print("Serial port for Valon: (%s) opened successfully." % port)
30       print("-----")
31       time.sleep(0.5)
32   # except self.SerialException as e:
33   #   print("Error opening serial port: (%s)" % e)
34
35   valonConnect = VSerialPort(port)

```

Future Work & References

- Chirped pulse implementation, improving Big O notation/optimization/settings, and finalizing GUI
- Integrating Tektronix Arbitrary Waveform Generator and generating waveforms via Python

References:

0: Oldham, James M., Chamara Abeysekera, Baptiste Joalland, Lindsay N. Zack, Kirill Prozumov, Ian R. Sims, G. Barratt Park, Robert W. Field, and Arthur G. Suits. 2014. 'A Chirped-Pulse Fourier Transform Microwave/Pulsed Uniform Flow Spectrometer. I. The Low-Temperature Flow System'. *Journal of Chemical Physics* 141.

1: R.M. Gurusinghe, N. Dias, R. Krueger, A. G. Suits. "Uniform supersonic flow sampling for detection by chirped-pulse rotational spectroscopy". *J. Chem. Phys.* 2016;144(20):200901.

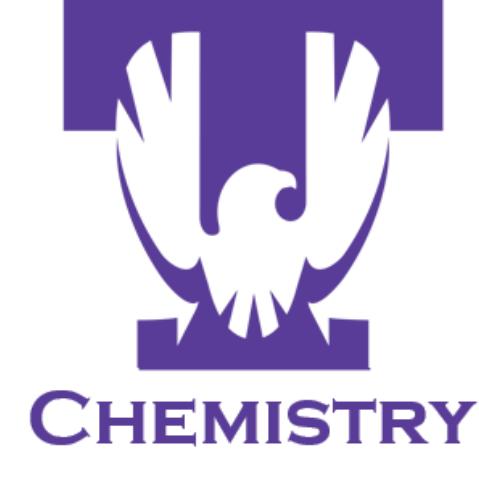
2: Park GB, Field RW Perspective: The first ten years of broadband chirped-pulse Fourier transform microwave spectroscopy. *J. Chem. Phys.* 2016;144(20):200901.

3: Abeysekera C, Zack LN, Park GB, Joalland B, Oldham JM, Prozumov K, Ariyasingha NM, Sims IR, Field RW, Suits AG. A chirped-pulse Fourier-transform microwave/pulsed uniform flow spectrometer. II. performance and applications for reaction dynamics. *J. Chem. Phys.* 2014;141(21):214203.

4: Huckauf, Dr. A. Dr. Jäger's Research Group. <https://www.chem.ulb.ac.be/~jaeger/index.htm>

5: Jovik Thomas, Oleksandr Sukhorukov, Wolfgang Jäger, and Yunjie Xu: "Chirped pulse and cavity based FTMW spectra of the methyl lactate - ammonia adduct: lock and key selectivity on internal rotation motions." *Angew. Chem. Int. Ed.* 52, 4402-4405 (2013).

6: Instrumentation Manuals and API documentation.



GRU LAB

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